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ARTIFICIAL NEURAL NETWORK METAMODELS OF STOCHASTIC COMPUTER SIMULATIONS

by

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Submitted to the Graduate Faculty

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in partial fulfillment of

the requirements for the degree of

Doctor

of

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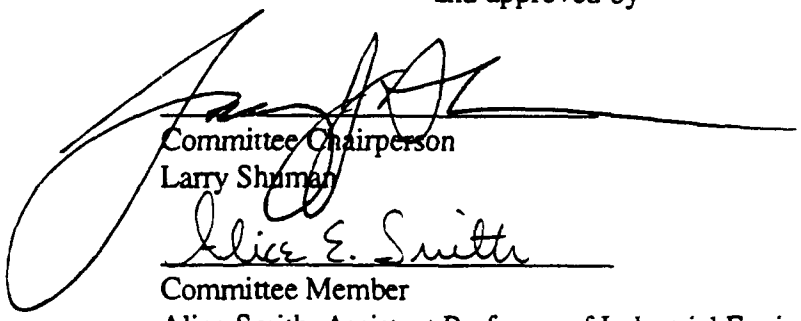

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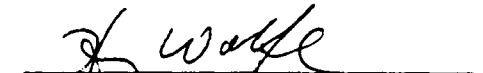

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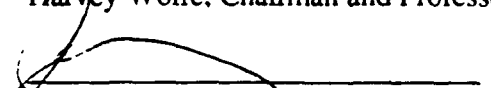

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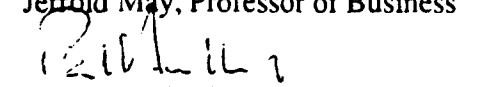

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I thank God for the privilege and honor of obtaining a Doctorate of Philosophy degree and I dedicate this document to the memory of my father, William Ralph Kilmer.

ABSTRACT

Signature_____

ARTIFICIAL NEURAL NETWORK METAMODELS OF
STOCHASTIC COMPUTER SIMULATIONS

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A computer simulation model can be thought of as a relation which connects input parameters to output measures. Since these models can become computationally expensive in terms of processing time and/or memory requirements, there are many reasons why it would be beneficial to be able to approximate these models in a computationally expedient manner. This research examines the use of artificial neural networks (ANN), to develop a metamodel of computer simulations. The development and use of the Baseline ANN Metamodel Approach is provided and is shown to outperform traditional regression approaches. The results provide a solid foundation and methodological direction for developing ANN metamodels to perform complex tasks such as simulation 'optimization', sensitivity analysis, and simulation aggregation/reduction.

DESCRIPTORS

Approximation

Artificial Neural Networks

Backpropagation

Computer Simulation

Confidence Intervals

Discrete-event Simulation

Estimation

Metamodeling

Multiple Linear Regression

Non-Linear Regression

Non-Parametric Regression

Prediction Intervals

Regression

Response Surface Methodologies

Sensitivity Analysis

Simulation Aggregation

Simulation Optimization

Simulation Reduction

Stochastic Simulation

Terminating Simulation

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NOMENCLATURE

(Bold type indicates a vector.)

C = Cost

GCBWT = General Care Bed Wait Time

ICBWT = Intensive Care Bed Wait Time

LABT = Laboratory Time

n = Number of replications of the computer simulation.

PM = Presentation Metho

$S_{Y_{ij}}$ = Standard deviation of Y_{ij}

$S_{\hat{Y}_{ij}}$ = Value of standard deviation of Y_{ij} predicted for $\mathbf{X_i}$.

T = Time

X = Generic input parameter setting of the simulation.

$\mathbf{X_i}$ = A particular input parameter setting, i.

XRAYT = X-Ray Time

Y = Generic simulation output measure.

Y_i = Simulation output measures. corresponding to $\mathbf{X_i}$.

Y_{ij} = jth element of the simulation output measures $\mathbf{Y_i}$.

$\hat{Y}_{ij}$ = Value of Y_{ij} predicted for $\mathbf{X_i}$.

1.0 INTRODUCTION

1.1 Problem Statement

The interactions and relationships among components of most real world systems are too numerous and complex for a human to recognize, much less understand. Thus, simplifications or approximations of systems, called models, are used to examine problems associated with the design, operation, maintenance, or modification of systems. Many of these models are implemented as computer simulations that accurately reflect much of the detailed interactions and activities of the components of the system. Essentially these computer simulations are mechanisms for converting system input parameters into output measures.[1]*

According to Box and Draper, there are two basic approaches to building a model of a system: mechanistic and empirical.[2] In the mechanistic approach, enough is known about the system to develop an explicit representation that tries to mimic its operation or processes. When the necessary information of the physical mechanism of the system is not known, then an empirical model that relies only on the observations of the inputs and outputs of the system can be constructed if there is enough observational data on the real system. For large, complex systems it is usually necessary to combine both approaches in order to realistically model the system. The development and use of both types of modeling approaches are depicted in Figure 1. As can be seen in Figure 1, the main difference between the two approaches is in the creation or development of the model, rather than the operation of the completed models.

*Parenthetical references placed superior to the line of text refer to the bibliography.

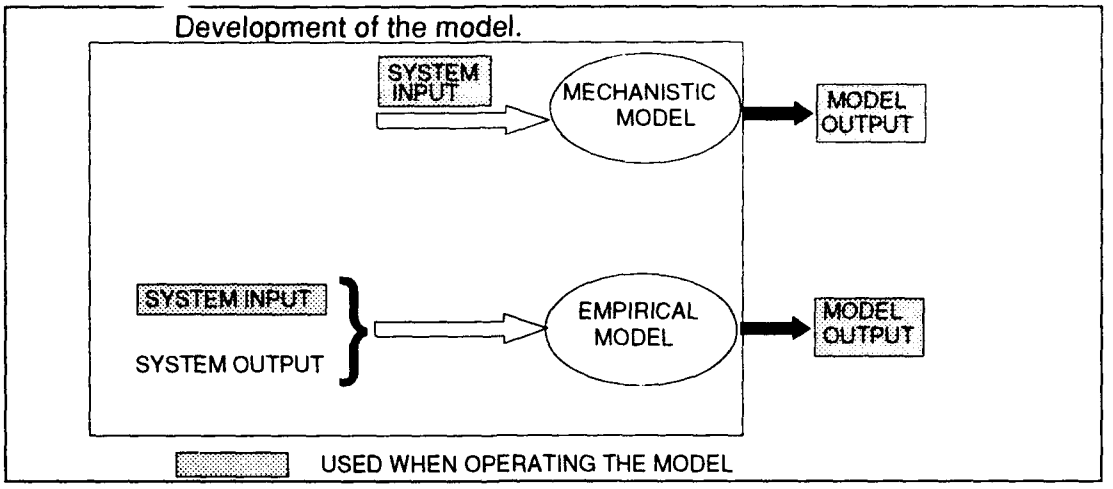


Figure 1 Mechanistic and Empirical Modeling Approaches

Mechanistic models are generally preferred over empirical models because of the clear and apparent connections to the real system. However, a major drawback to many mechanistic models is that they can be extremely slow to operate, thus requiring tremendous amounts of computer resources.

Consider a fairly common situation where a slow but accurate mechanistic computer simulation model of the system exists and there is very little observational data of the real system. One approach to resolving this situation would be to build an empirical model using the data from the real system. However the lack of real system data would probably produce a poor empirical model. Another approach would be to take advantage of the existing mechanistic computer simulation to obtain data for use in developing an accurate and fast operating empirical model. In this approach the empirical model is actually a metamodel (i.e., a model of the computer simulation model), rather than a direct model of the system.

For more than twenty years, metamodels based primarily on response surface techniques, have been used to examine computer simulations. Most response surface methods currently use linear regression to build empirical models of computer simulations.(3) The central idea of this research is to use Artificial Neural Networks (ANN) to construct the empirical model of the computer simulation, since ANN are essentially capable of performing non-parametric, nonlinear regression.(4) Figure 2 shows the metamodeling approach and terminology for the regression and ANN empirical models.

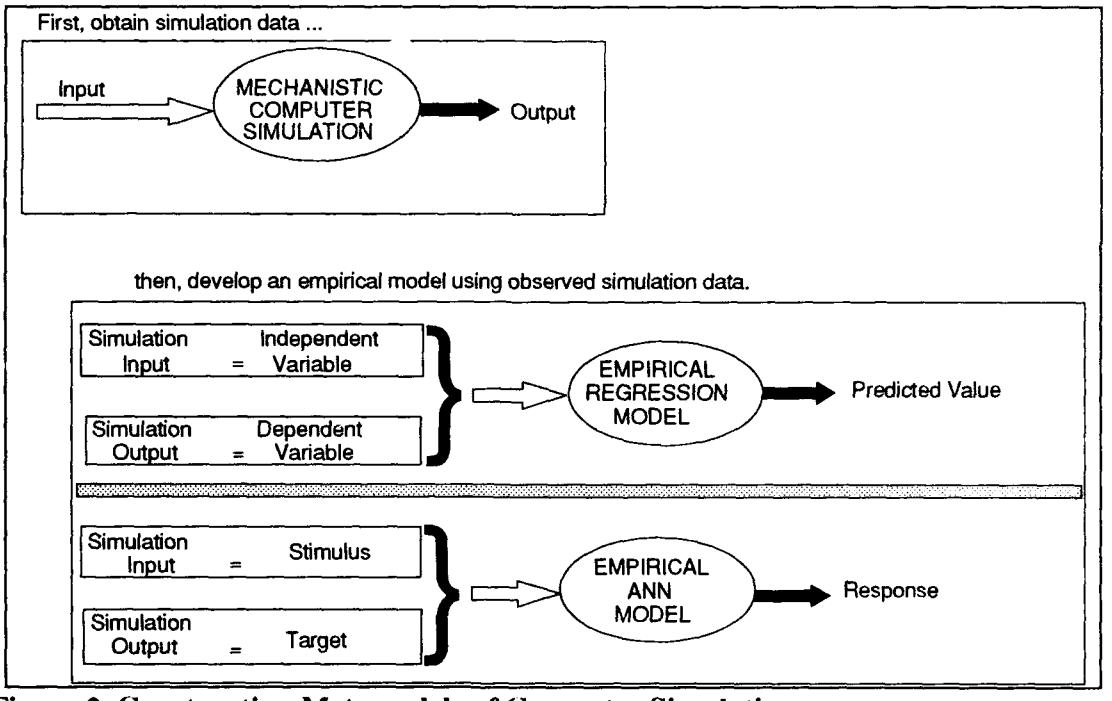


Figure 2 Constructing Metamodels of Computer Simulations

While beyond the scope of this dissertation, the ultimate goal is to use ANN approximations in lieu of mechanistic computer simulations in performing such complex and time consuming advanced tasks as simulation 'optimization,' sensitivity analysis, and simulation aggregation/reduction. In order to attain this goal, it is necessary to study and

understand the limitations and strengths of ANN approximations to perform the most elementary, yet fundamental, tasks of simulation. Computer simulations are used to perform the following basic tasks:

To predict the output measure of a system for a given input parameter setting.

To determine the output measure's average value and variance for a given input parameter setting.

To determine if the output measure for a given input parameter setting is significantly different than a specified value of interest to a decision maker.

To determine sensitivity of the output measure to change in the input parameters.

The problem that this dissertation addresses is how to perform these basic simulation tasks with ANN approximations of a computer simulation rather than performing these tasks directly with the computer simulation. This dissertation provides the foundation for using ANN approximations of a computer simulation to perform advanced simulation tasks.

1.2 Importance of Computer Simulation

Computer simulation has been identified in surveys as the most widely used tool of industrial engineers and management scientists.[5] Computer simulation has several advantages over other techniques for examining systems. Often computer simulation is the only means for examining a real world system. Sometimes, this is due to the size and complexity of the system, since some systems cannot be accurately represented by an analytical mathematical model. On other occasions, this is due to the fact that the system does not exist or the conditions under which the system will operate are too dangerous,

costly or infrequent to permit direct experimentation with the system. Examples include the United States space station, conducting nuclear war, and designing the tunnel under the English Channel between England and France. Other advantages of simulation include the ability to have complete control over the experimental conditions and to study system operation over long time horizons.[6]

There are a wide variety of application areas such as the military, service industries, manufacturing organizations, and transportation companies throughout the world that make extensive use of computer simulations. For example in the military, computer simulations are used to conduct training for individual soldiers in tanks and aircraft, examine operation plans and force structures, as well as to evaluate future weapons systems.[7] The main reason these computer simulations are being used is that they provide realistic results and, in many cases, provide them at a lower cost than alternative approaches.

1.3 Problems with Computer Simulations

Simulation models often are expensive to develop and use, in terms of personnel, time, and other resources. Sometimes too much confidence is placed on the results of a computer simulation simply because these results were produced by a large, very detailed computer program. Computer simulation models also have the opposite type of problem: the results are not accepted because decision makers consider the large, detailed computer program to be a 'black box.' Additionally proper interpretation of computer simulation output usually requires training and experience in using statistical methods to prevent

people from doing such things as interpreting the results of one replication of a stochastic simulation as being 'the answer.'[8]

Simulation is typically considered a 'means of last resort' due to the cost of building, verifying, validating, and using simulation models. Hillier and Lieberman succinctly state: "... simulation is a slow and costly way to study a problem."[9] The longer it takes to run a computer simulation on a particular computer platform, the more difficult it is to perform the necessary checks involved with verifying and validating the computer simulation. Another problem is that these simulations can grow so large that they exceed the memory capacity of the computers, or the commercial modeling languages, that are available to the users of the simulation. Even after expending the resources to obtain a valid model, slow response time or large memory requirements, caused by the complexity of the computer simulation, can prevent, or seriously impede, such activities as performing quick turn-around studies, sensitivity analyses, model aggregation, and simulation 'optimization'.

1.4 Need for Better Approximations to Computer Simulation Models

For more than 30 years, computer simulation models have been used to predict how systems would perform under certain conditions. Many of these models have been accepted as valid representations of the underlying system because the model accurately reflects the behavior of the system as it operates over time. Over the past several years, in combination with response surface methods, these models have also been used, not only to predict the behavior of a system for a given set of input parameters, but also to prescribe

the input parameter settings that would result in good or 'optimal' output values of the model with respect to the particular problem of concern.

However, because of the detailed information that is necessary for precise prediction over time, it is difficult to find 'optimal' solutions to these predictive models. What makes it so difficult to 'optimize' a predictive model is that they are usually computationally expensive and have a very large number of possible solutions in the input parameter space. In 1989, Jacobson and Schruben state that "Although there has been a significant amount of research in the area (simulation optimization), no general approach has been developed into an efficient and practical algorithm."[10] This situation still holds five years later. Thus, there is a need to reduce the computational burden of computer simulations to permit identification of good solutions for designing, operating, and maintaining large, complex systems.

Typically, computer simulation 'optimization' is currently conducted through response surface methodologies (RSM) using regression model approximations of the computer simulation. The regression model approach in RSM has been used successfully for such purposes as performing sensitivity analyses within a limited region of the input parameter space, determining constraint satisfying solutions, and simulation 'optimization'.[11] The regression model approach has not been used to perform global estimation or approximation. The regression model approach has typically been limited to first- and second-order regression models.[12] Myers, Khuri and Carter state: "There appears to be some need for the development of non-parametric techniques in RSM. Most of our analytic procedures depend on a model. The use of model-free techniques

would avoid the assumption of model accuracy or low-order polynomial approximations and, in particular, the imposed symmetry associated with a second-degree polynomial."(13)

The possible approaches to solving the problems caused by the computational burdens of computer simulations are to obtain more powerful hardware, rewrite the computer simulation to be more computationally efficient, or to develop a small and/or fast approximation to the computer simulation. In many cases, the first and second approaches have already been taken or were impractical due to a lack of capital funds or the ability of available simulation programmers. In addition, if a computer simulation has achieved a high degree of user acceptance due to extensive verification and validation efforts, there is a certain amount of reluctance to make significant modifications to the computer simulation. Thus, the third approach, approximating computer simulations, needs to be examined.

As Simon puts it, ***"When our goal is prescription rather than prediction, then we can no longer take it for granted that what we want to compute are time series. ... But facts must be faced. Intelligent approximation, not brute force computation is still the key to effective modelling."***(14)

1.5 Using ANN to Approximate Computer Simulations

One possible non-parametric approach, which is the focus of this research, is to have an artificial neural network "learn what the computer simulation knows" by training on the inputs and outputs of the computer simulation. As Padgett and Roppel state: "Neural networks in all categories address the need for rapid computation, robustness, and

adaptability. Neural models require fewer assumptions and less precise information about the systems modeled than do some more traditional techniques."[15]

The idea of using an ANN to approximate a computer simulation may initially seem routine to researchers with an extensive background in neural networks. The reason for such an assessment is that there are many examples of researchers using computer simulations in order to obtain data to train their networks.[16,17,18] The majority of these cases involved research in modifying or developing new ANN methodologies, techniques, or procedures. Thus, instead of expending valuable time and effort to obtain data from a real system, these researchers obtained their data from computer simulations that were built with the sole purpose of "feeding" an ANN. However, while it might be fairly trivial to build a computer simulation to provide training data to an existing ANN, this does not mean that it will be easy to build an ANN that will be able to receive and learn the relationships of an existing, complex stochastic computer simulation.

ANN have been used quite extensively to perform function approximation. However, computer simulations of the type examined in this dissertation are more difficult to approximate. There are three major differences between using ANN to approximate stochastic simulations and using ANN to perform ordinary function approximation. First, due to the stochastic nature of the computer simulation, a given set of inputs yields different outputs, thus compounding training. Second, training and testing data are computationally expensive to generate, and therefore must be leveraged. Third, training and testing data are usually designed; i.e., are not randomly chosen from the problem domain.[19]

While the largest payoffs for a computer simulation approximation tool are likely to be in the complex areas of simulation optimization, sensitivity analysis, and model aggregation, it is necessary that a solid foundation be established for using the approximation tool, either in lieu of, or in conjunction with, the computer simulation. Therefore, it is essential to know how to use the approximation tool to perform the most rudimentary computer simulation tasks.

The major contribution of this dissertation is that it provides an empirically based methodology and discusses the capabilities, limitations, advantages and disadvantages, for using ANN approximations of computer simulations to perform the basic simulation tasks of prediction and comparison of alternatives. An additional contribution is the development of the foundation for using ANN approximations of computer simulations for performing advanced simulation tasks.

1.6 Overview of the Dissertation

This dissertation contains eight chapters and three appendices. Chapter 1 provides a general introduction to the problem of approximating computer simulations with Artificial Neural Networks. A detailed literature review of computer simulation, approximation theory, and approximation approaches is given in Chapter 2. The research issues, methodology and tools used to conduct the research are detailed in Chapter 3. Chapters 4 and 5 cover the description, experiments, results and lessons learned from the problem used to develop the baseline Artificial Neural Network metamodel approach. Chapter 6 delineates the baseline ANN metamodel approach. Chapter 7 provides the results of applying the baseline ANN metamodel approach on a demonstration problem,

specifically a simulation of an emergency department. Chapter 8 contains the summary and conclusions derived from the research effort as well as areas for potential future research. The appendices and bibliography follow Chapter 8.

1.7 Restrictions of the Research

Since the focus of this research effort is on developing a tool that could be used to approximate a computer simulation, it is assumed that the topology of the internal relationships and procedures within the computer simulation have been determined and will not be modified (i.e., the computer simulation to be approximated has already been finalized, verified, and validated). Therefore, this research did not address problems associated with building computer simulation models. Nor does it deal in detail with problems of verification and validation of computer simulation models. Further, it is assumed that only the values of the input parameters that are provided to the computer simulation can be changed.

The prediction of output values will only be done for those output values determined at the termination of the simulation. Predicting a series of values of the output measure over time is a subject for future research efforts.

This research only examined terminating, stochastic, discrete-event computer simulations. A description of these terms is provided in Chapter 2. This research focused on the type of computer simulation typically used for addressing industrial engineering/management science/systems analysis problems. However, this same approach should be generalizable to other areas.

This research uses feedforward, multi-layered, fully connected artificial neural networks trained via the backpropagation learning algorithm. The reasons for having chosen such a network paradigm are discussed in Chapter 3.

1.8 Summary

This chapter provides an introduction to the problem of interest. Specifically, it presents an overview and demonstrates the need for approximating computer simulations with artificial neural networks. A brief discussion of the topics of computer simulation and its importance, modeling approaches, and the fundamental idea of using the results of a computer simulation to provide data for building an empirical model of a system are also provided. An overview of the dissertation document is provided as well as a discussion of the restrictions of the research effort.

2.0 LITERATURE REVIEW

2.1 Computer Simulation

Simulation has been defined by Pegden as: "the process of designing a model of a real system and conducting experiments with this model for the purpose of understanding the behavior of the system and/or evaluating various strategies for the operation of the system."[20] Just about anything can be simulated on a computer. Computer simulations range from models of simple mathematical functions, such as $y = \sin(x)+4x$, to complex models of the universe.

There are various ways that computer simulations can be classified. Law and Kelton provide a way to categorize computer simulations using four dichotomous characteristics:[21]

(1) *Deterministic versus Stochastic*. Deterministic simulations provide a unique solution for a given input, no matter how many replications are performed, whereas the stochastic simulation contains probabilistic elements, and therefore provides only an estimate of the output variable.

(2) *Static versus Dynamic*. A static simulation is a representation of a system where time does not have an impact, while a dynamic simulation is affected by the passage of time within the simulation.

(3) *Discrete versus Continuous, or Mixed.* This is a characteristic of dynamic computer simulations. In discrete simulations, the variables can change only at specific points (at most a countably infinite number of points) in time, whereas in continuous simulations, the variables change continuously (i.e., without a break or jump between values) over time. A mixed simulation contains some variables which are discrete and some which are continuous.

(4) *Terminating versus Non-terminating.* This is a characteristic of dynamic computer simulations. A terminating simulation is one where there exists a natural termination criteria for the system that is being simulated. A non-terminating simulation does not have a natural termination criteria and so analytical or heuristic methods are used to determine when to stop the simulation.

To a great extent the answer to the question "what is computer simulation?" depends on the respondent. Each area of specialization such as aeronautics, chemistry, economics, nuclear engineering, medicine, physics, or warfare has its own repertoire of computer simulation models that are used in research and applications. Due to the characteristics of the problems in each area, certain types of models will perform better than others and will, therefore, tend to dominate a field of specialization. For instance, in the fields of operations research, systems analysis, and industrial engineering, which developed concurrently with the use of computers, Quade states "... simulation is the process of representing item by item and step by step the essential features of whatever it is we are interested in... ."[(22)] Thus, researchers in these fields tend to think of computer simulations as mechanistic models of systems. In this dissertation it is assumed that the term computer simulation means a mechanistic, stochastic, dynamic, discrete, terminating

simulation since the majority of simulations in the field of industrial engineering are of this type. Discrete-event models are by implication dynamic as well as discrete. Thus, this research considers mechanistic, discrete-event, stochastic, terminating computer simulations.

In the past, many organizations had the luxury of making decisions on the basis of studies of long duration, and thus, the computer simulation models that were used in conducting these long duration studies did not need to be very fast. This situation was especially pronounced for examinations of very large and complex systems such as rain forests, space stations, and military operations. Today, with more managers becoming comfortable with the use of computers and computer simulation models, as well as the increasing pressures of global competition, there is a greater demand to have results from computer simulations in a shorter amount of time.[23-28] If the computer simulation is too slow, as can typically be the case when portions of the simulation employ large Monte Carlo modules to generate responses, then the results may not be available in time to assist the decision maker.

Computer simulations are also used to perform sensitivity analysis for large complex systems.[29] Sensitivity analysis means being able to answer the "what if" questions that a decision maker might ask concerning the issues that are being investigated. This typically requires making many different runs and replications of each variation of the input parameter settings. Thus, if the computer simulation is slow, the amount of sensitivity analysis that can be performed will be limited. Sensitivity analysis of computer simulations currently can be very expensive.[6]

Computer simulation models for very large, complex systems are sometimes constructed by building a series of models for different system components, usually called modules, and then linking them together to form an aggregate model of the system. While each of the individual modules might perform quite effectively, the aggregate model might be very slow and possibly exceed the memory requirements of the computer. Thus, there is a need for model reduction techniques to make the larger and more computationally expensive modules more efficient.[30,31]

Over the past several years, computer simulation models have also been used, not only to predict the behavior of a system for a given set of input parameters, but also to prescribe the input parameter settings that would result in "optimal" output values of the model with respect to the particular problem of concern.[32] It should be noted that what is meant by an "optimal" solution in the context of simulation is really closer to a "superior" solution rather than the "best" solution interpretation typically found in the field of optimization. However, because of all the detailed information necessary for precise prediction over time, it is difficult to find optimal solutions to these models. Just as humans become overloaded with information about the real world when it is necessary to predict the behavior of such systems, these computer simulation models may be processing too much irrelevant information when it comes to prescribing solutions to posed problems.

2.2 Artificial Neural Networks

A neural network is a computational mechanism that achieves power and flexibility through the use of parallel and sequential processing elements. The field of neural networks is also known as parallel distributed processing or connectionism.[33] The initial

focus of neural networks was, and the work of many current researchers is, on developing artificial structures that model the actual operation of a biological brain. Many other research efforts, including this one, make no claims about their neural networks reflecting features of how the brain actually operates. To emphasize the distinction, the latter group of networks are referred to as artificial neural networks (ANN).

The earliest work in neural networks was reported in 1943 by McCulloch and Pitts who developed networks which today are called "McCulloch-Pitts nets." While these nets are very simple by current standards, the noted mathematician John von Neumann proved that redundant McCulloch-Pitts nets can perform arithmetic calculations with high reliability, but not necessarily as efficiently as traditional sequential computing algorithms.[34] Currently, there are many different kinds of neural networks with various architectures and learning algorithms that are used for many different purposes in a wide variety of applications.[35,36] Cheng and Titterington provide an excellent discussion of neural networks from a statistical perspective by examining the similarities and differences between traditional statistics and artificial neural networks.[37]

It should be noted that in the field of neural networks the term "computer simulation" has typically been used in two different ways. The more prevalent use is to indicate a software implementation of an ANN on a sequential processing computer to distinguish it from a hardware implementation on a parallel processing computer or chip.[38] A secondary use is to describe one of the mechanisms for obtaining data to test an ANN methodology, technique, or structure. This is typically done when it is difficult or impossible to obtain real world data. This secondary interpretation is closer to the manner in which the term "computer simulation" is used in this research.

Even though there seems to be a wide variety of objects that claim to be artificial neural networks with differing terminology, the following definition appears to encompass most, if not all, of the various artificial neural networks. An artificial neural network can be defined as a directed graph consisting of nodes (or units) that are connected in some manner with the following properties[39]:

1. Each node i has an associated state variable with activation level, A_i.
2. Each connection between nodes i and j has a real-value weight, w_{ij}.
3. Each node i has an associated real-value bias, V_i.
4. Each node i has a transfer function, $t(A_j, w_{ij}, V_i)$.

The transfer function is usually non-linear and is used to determine A_i, the new state variable, based on the summation of all inputs into node i: the state, A_j, of all nodes j connected into node i; the weights, w_{ij}, of the connections coming into node i; and the bias of node i, V_i. Thus, $A_i = t(A_j, w_{ij}, V_i)$. A depiction of a typical node which in this example has two inputs is given in Figure 3.[40] The activation level for the node in Figure 3 is given in equation 2-1.

$$A_i = t\left(\left(\sum_{j=1}^{2} w_{ij} \times A_j\right) + w_{io} \times V_i\right) \qquad (2\text{-}1)$$

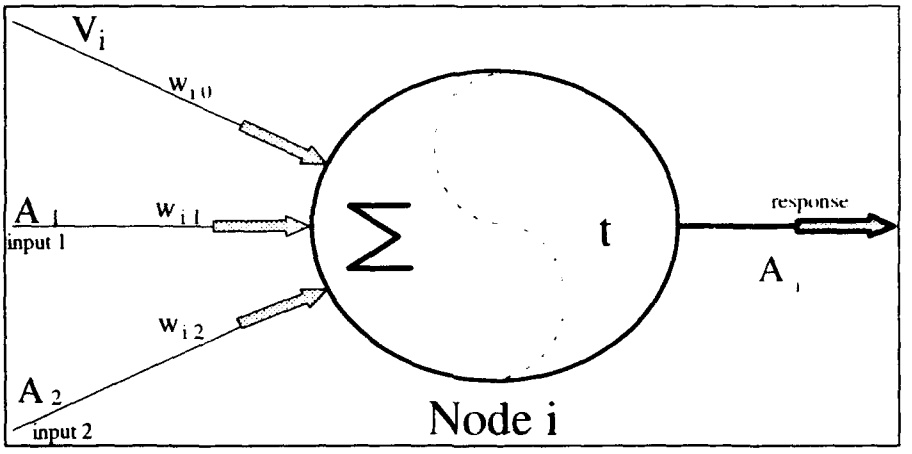


Figure 3 A Typical ANN Node

While there is very little that an individual node can do, by combining many different nodes, ANN are capable of approximating complex functions. The nodes of an ANN are typically placed into one of three types of layers. The input layer only receives stimuli or information from outside the network. The output layer is used to provide results from the network. The hidden layer(s) is used to permit different operations to be performed on the data. The hidden layer derives its name from the fact that it is invisible to the world outside of the network. In other words, the hidden layer neither receives nor transmits any information directly outside of the network. Some types of ANN do not use a hidden layer of nodes. If, for all layers of the network, all the nodes in one layer of the network are connected to all the nodes in the succeeding layer of the network, then the network is called a fully connected neural network. Following the convention used in Zurada, only the hidden and output layers are counted when describing the number of layers in the network.(41) For example, a network with an input layer, two hidden layers and an output layer would be referred to as a three layer network.

One way to characterize networks that are organized into layers is with regard to the direction of the flow of information between the layers of the network. If the flow of

information about the state of the node cannot be fed back to itself either directly or indirectly through other nodes, then the network is called a feedforward network. Otherwise, the network is called a feedback network.[42] Figure 4 graphically depicts a fully connected, multi-layered, feedforward ANN [43]

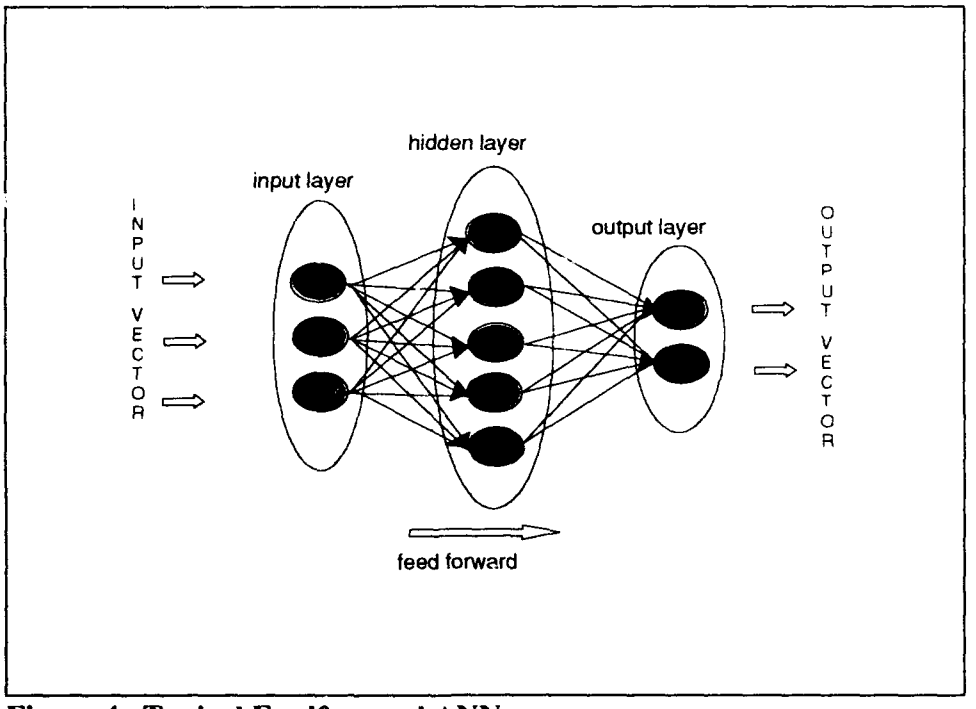


Figure 4 Typical Feedforward ANN

Researchers have developed many different approaches for "teaching" an ANN to "learn" the relationship between the inputs and outputs of a system. The outputs of the system are typically referred to as "targets" in the connectionist literature. In the situation called "supervised learning," input and target pairs of data are available for the system of interest. The data is shown (i.e., provided) to the network one pair at a time to provide an opportunity for the network to "learn" the relationship that exists between the input and target data. In this research, a training point consists of both the input vector and the corresponding target vector. The information about the outside world is provided to the

ANN through the activation values of the input and output nodes (i.e., through the A_i). The knowledge of the network is stored in the weights of the network (i.e., in the w_{ij}). Typically, a network starts in a randomized state of initial weights and is trained iteratively until reaching an "intelligent" state.

A very popular, nearly "standard", training mechanism is called "backpropagation" or the "generalized delta rule." First developed by Werbos[44] and publicized widely by Rumelhart and McClelland,[45] the generalized delta rule is usually used for feedforward, fully-connected networks and is divided into two stages. In the first stage of training, as is depicted in Figure 5, one input data vector is presented to the input nodes of the network, and processed in a forward direction through the network with the states of the nodes being passed from one node to the next until the output nodes have newly assigned state values or activation levels, called the response vector. The response values of the output nodes are then subtracted from the corresponding target values, resulting in an error value associated with each output node.

The second stage of training, depicted in Figure 6, propagates the squared error from each output node backwards through the network, and adjustments are made to the weights and thresholds of the network using gradient descent to reduce the size of the total squared error of the network.[45] Selecting a new training point and applying both training stages to the new training point continues until the training stoppage criteria is achieved. Typical training stoppage criteria include convergence for all of the training data to less than a pre-specified error level or after performing a pre-determined, large number iterations through the training data.

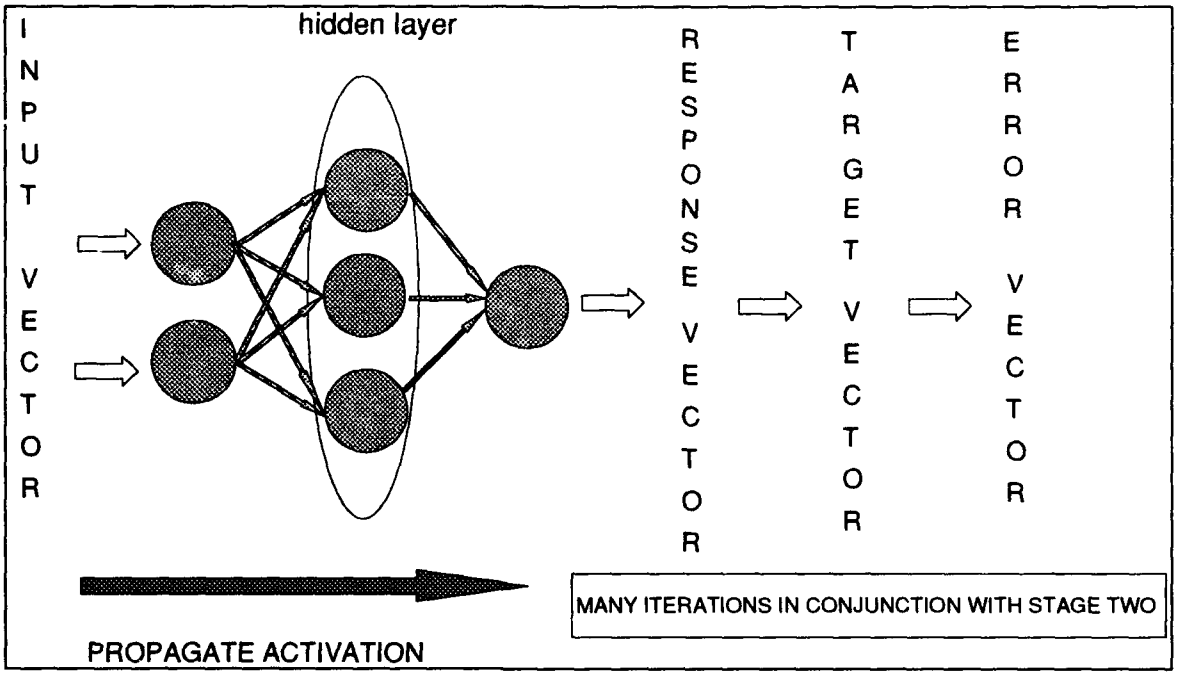


Figure 5 ANN Training: Stage One

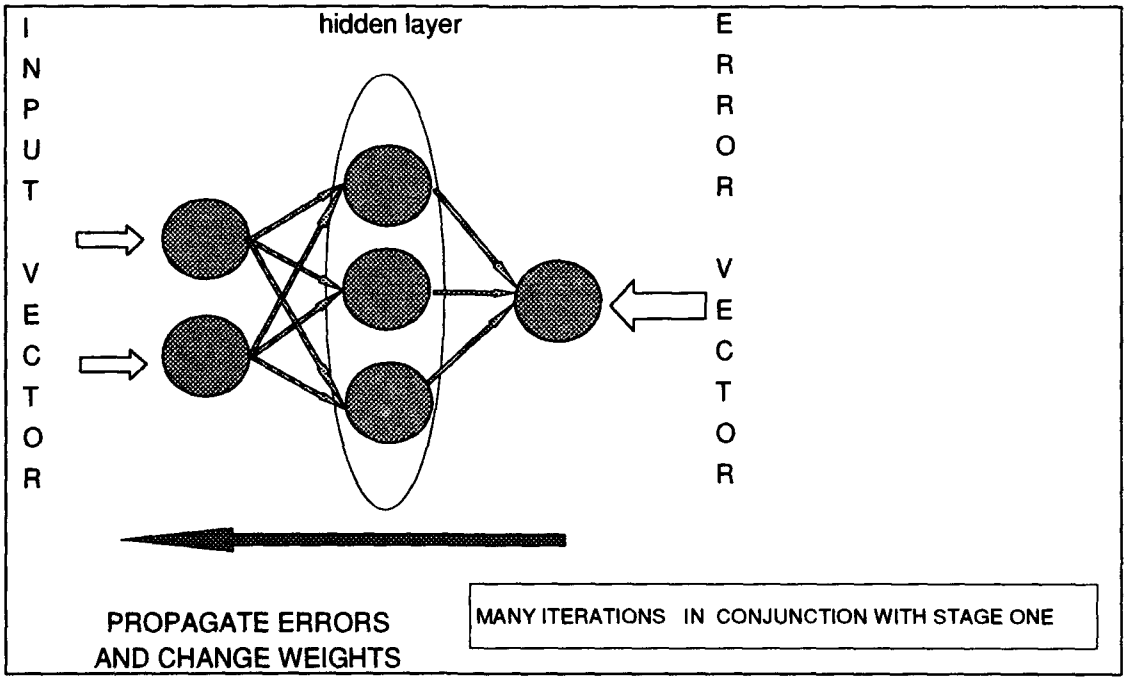


Figure 6 ANN Training: Stage Two

Once the training is concluded, a check on the generalizability of the trained ANN is usually performed by testing another set of data, distinct from the training set, using the weights determined by the training procedure. This test is conducted in the exact same way as the first stage of training, but consists of only one pass through the network, as depicted in Figure 7. The input data is provided to the network and the activations are propagated only one time for each input data vector and the resulting response is compared to the target to obtain the error of the ANN on each test point.

Finally, as is depicted in Figure 8, the trained network is used in an operational mode to obtain predicted responses to input vectors for which target vectors are not available. This is similar to testing the network in that there is only one pass for each point in the data set. However, in this case there are no target vectors to use to determine the accuracy of the ANN.

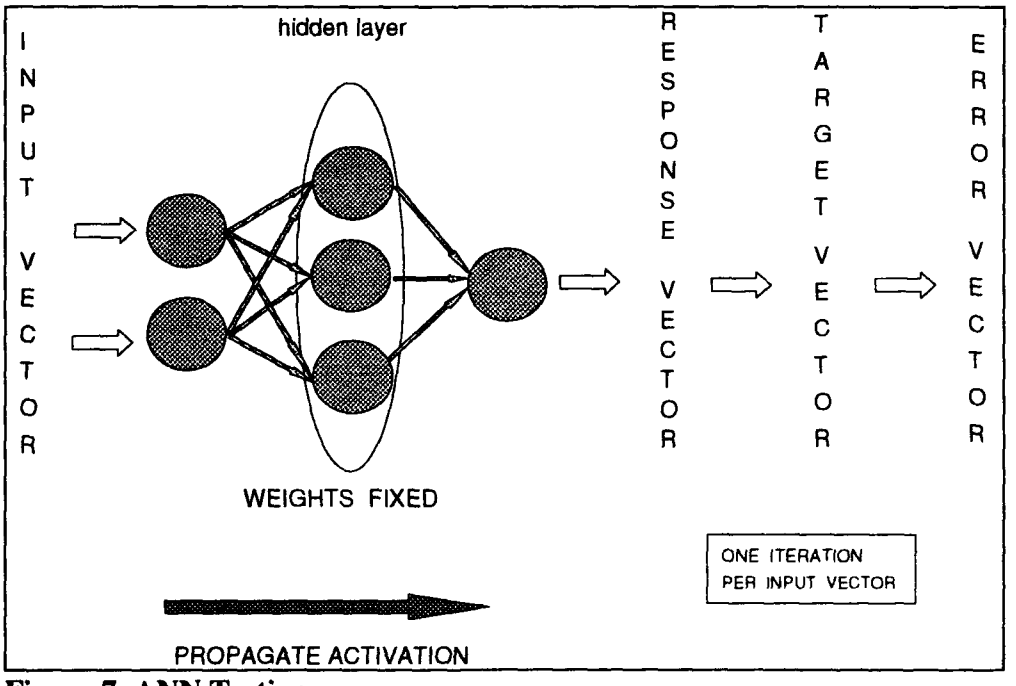


Figure 7 ANN Testing

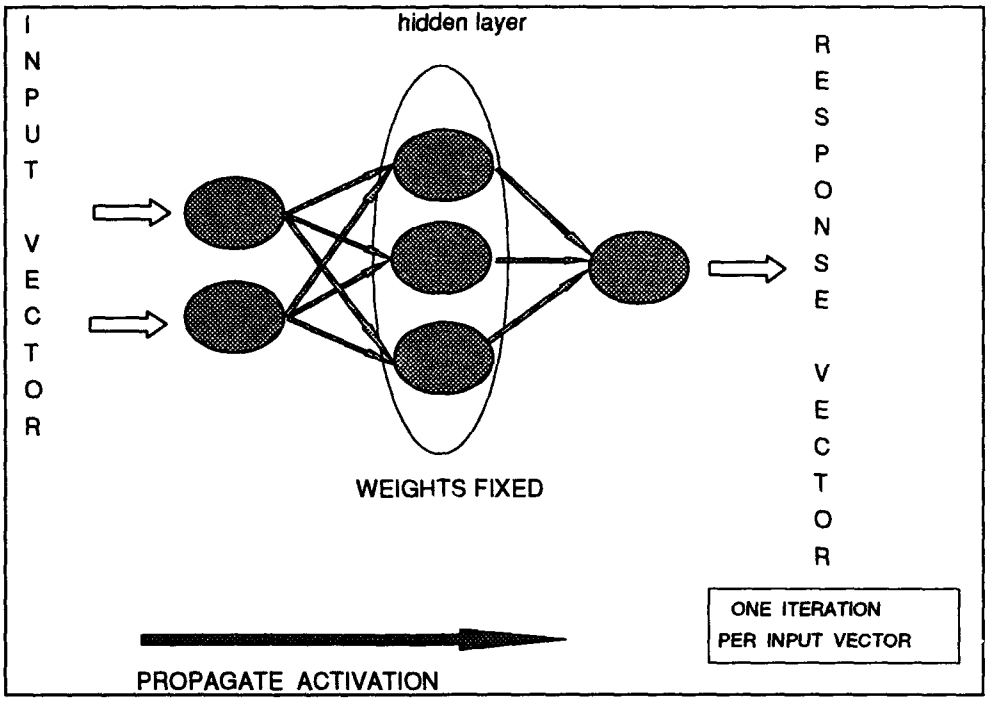


Figure 8 ANN Operation

This research used the backpropagation method of training feedforward, fully connected ANN for the following reasons. First, several researchers have already successfully used these networks for performing arbitrarily well the task of approximating continuous functions and have shown that they are in fact "universal approximators."(46-54) Second, the widespread availability of software for performing backpropagation will enable computer simulation researchers unfamiliar with ANN to quickly and easily use and apply the results of this research effort. Third, it has been shown that backpropagation is equivalent to the Robbins-Munro stochastic approximation procedure for solving the nonlinear least squares regression problem.(4) Fourth, the focus of this research is not on finding the "best" ANN for approximating computer simulations, but on determining how to use ANN to approximate computer simulations and discovering the advantages,

disadvantages and limitations of such an approach. Therefore, to emphasize that this is not a study of ANN methodology, but rather a study of how to use ANN to approximate computer simulations, a well-accepted, conceptually easy to understand, "standard," ANN that may not be the most efficient at continuous function approximation was used.

There are two major drawbacks of the backpropagation algorithm that have caused researchers to examine alternative training procedures. The first problem is possible convergence to local minima rather than the global minimum of the error surface and the second problem is computational expense and the consequent time to train using backpropagation.[55] It was once conjectured that backpropagation trained networks would always converge to the global minimum. It has been shown that this is true in many practical applications but there are cases when they do converge to local minima because it is essentially a gradient descent procedure.[56] One of the reasons that backpropagation is computationally expensive is that the network architecture, in terms of the number of hidden nodes, is determined on a trial and error basis. Much of the research has been directed at examining various methodical procedures. One approach used in this research is to start with the smallest possible network, train that network, add another node to the network, and repeat the process until performance begins to worsen. This simple approach and other more sophisticated techniques such as adding or trimming hidden nodes during training are discussed by Hush and Horne.[57] Other researchers have developed such modifications to the traditional backpropagation training algorithm as Quickprop,[58] RPROP,[59] Double BackProp,[60] and others based on sophisticated non-linear optimization procedures.[61-65]

Other neural network approaches to function approximation have also been developed. One of the most promising of these alternatives to backpropagation is Radial Basis Function (RBF) neural networks. Poggio and Girosi have published several articles on Radial Basis Function artificial neural networks that have the best approximation property for continuous multivariate function approximation.[51,52,66] However, there is no guarantee that these networks will also have the best approximation property for discrete multivariate functions. Also the RBF neural networks are not nearly as well known as the backpropagation neural networks. For these reasons the RBF neural networks are not examined in this research. They do appear to hold promise especially in their ability to provide confidence interval estimates for their responses.[67]

This research used networks with two hidden layers even though it has been shown that one hidden layer networks can approximate any continuous function.[68,69] However, one hidden layer networks may require an infinite number of nodes to be able to approximate a given function. In contrast, two hidden layer networks do not require the assumption of the availability of an infinite number of hidden nodes[70] and those networks can solve most real world approximation problems with only the two hidden layers.[71]

According to Padgett and Roppel: "A neural network can be thought of as an advanced simulation technique incorporating ideas from many fields and capitalizing on modern-day parallel processing and microelectronics capabilities."[15] Since there are researchers who are examining the use of the neural network techniques for performing simulation,[72] it is obvious that issues such as when should the ANN approach be used to directly perform the simulation and when should the ANN technique be used to

approximate another simulation model, will arise. This research will provide information that will be helpful in addressing these types of issues.

Four examples in the literature have been found where an ANN was constructed for the purpose of approximating or estimating the results of a computer simulation model. The first example, by Fishwick, found that a backpropagation trained neural network was not as effective as a regression model in approximating a deterministic computer simulation. However, it should be noted that the author appears to have only trained one network and did not change any of the default settings of the neural network software package used in the research.(73) In the second example, Pierreval and Huntsinger examined the issue of whether the data used to train neural networks as metamodels of computer simulations should be factorial design points or randomly generated points. While randomly generated points seemed to produce better networks in terms of generalizability to test set data, it appears that this was due mostly to the fact that the random training sets were larger than the factorial design training sets.(74)
In the third example, Badiru and Sieger reported good results when using a neural network trained on economic models.(75)

In the fourth example, Hurrion showed that "it is possible to fit a neural network to model the generalized response of parameter changes in a visual interactive simulation."(76) The simulation was a stochastic, discrete event, terminating model of a train depot developed as a demonstration of "visual interactive simulation."(77) A random number of trains arrived at the depot each day to receive coal and the depot remained open until all of the trains had departed the depot. The output from the simulation was the length of time the depot remained open each day.

Hurrion conducted two experiments in approximating the simulation of a coal depot with a backpropagation trained fully connected feedforward artificial neural network. The first experiment was designed to show that a simulation could be approximated by a neural network. Five different input factors were chosen with each factor having three different levels. The simulation was replicated nine times at each of the 3^5 (i.e., 243) design points and the mean and variance, of the time the coal yard remained open was calculated over the nine replications. The 99% lower and upper confidence limits for each of the design points were also calculated. Artificial neural networks were then constructed to try to approximate the simulation results of mean, lower confidence limit and upper confidence limit of the time the coal yard was open. The network architecture that was able to learn the relationships between the input factors and the output responses had five input nodes, one for each of the input factors, thirty hidden nodes in each of two hidden layers, and three output nodes. The output nodes corresponded to the mean and the two confidence limits. The result for the training set was that the neural networks prediction of the mean always fell within the original simulation's 99% confidence intervals. In addition, the mean predicted by the neural network for a test set of six different combinations of input parameters that were not included in the training set, also fell within the 99% confidence intervals of the original simulation. The test set was small in comparison to the training set and all of the values were internal to the values included in the training set. This experiment showed that "it is possible to fit a neural network to obtain the general response of a simulation's output over a wide range of input factors."(78)

Hurrion also demonstrated an incremental approach of building a series of neural network approximations to a computer simulation, where each neural network

approximation was used to guide the selection of future points for simulation and addition to the training set. One purpose of this demonstration was to show that the neural network approximation could be used as a tool for facilitating the interaction between the developer and client of a computer simulation model by providing very quick replies to "what if" questions posed by the client.[76]

In addition to using ANN to approximate the output of a system for a given set of input parameter values, some work has demonstrated the potential for using ANN to performing inverse mappings (i.e., for a given set of system output measures predict the corresponding system input values).[79-81] In one case, an approach using backpropagation trained ANN to learn the inverse of the simulation of a manufacturing facility job shop was demonstrated.[82] In this example, the simulation had three input parameters that were varied and four output measures that were generated by the simulation. The three input parameters were the number of resources in each of three separate work centers of the job shop. The four output measures were mean tardiness time, mean flow time, mean resource utilization and workload completion time.

Two neural network architectures were used to learn the inverse of the simulation. Both neural networks had four input nodes corresponding to the output measures of the simulation and three output nodes corresponding to the input parameters for the simulation. One network had one hidden layer of eight nodes and the other network had one hidden layer of fifteen nodes. The approach consisted of starting with a small initial training set of five (output, input) training pairs. Once the network learned the small training set, the network was used to predict the inputs to the simulation that would generate a set of desired output measures.

The simulation was then run at the predicted input parameter settings to obtain another observation of simulation output measures. The inputs generated by the ANN and the new outputs from the simulation were then added to the training set and used to train a new neural network. This iterative procedure continued until the outputs from the simulation that used the inputs generated by the ANN matched the desired outputs of the simulation.

The preliminary results of this example showed that the approach has promise since both of the networks showed improvement in the output measures of the network-predicted input parameter settings of the second iteration over the first iteration of the procedure. As Chryssolouris et al. point out, the procedure of using computer simulations to provide the data for training artificial neural networks has the potential for reducing the number of simulations required when using simulation to support manufacturing system design.[82]

One example was found in the literature in which an artificial neural network was used to replace a portion of the rule base of a discrete event computer simulation.[83] A portion of the expert system module of the U. S. Army's Combined Arms and Support Task Force Evaluation Model (CASTFOREM) was used off-line to train an ANN to make classification decisions. The decision that the ANN was trained to make was when the Orange forces should withdraw when being attacked by the Green forces. The inputs to the ANN were the number of Orange losses, number of Green losses, and the distance between the two forces. The output of the ANN was a classification of either to withdraw or not withdraw. The ANN was trained with the backpropagation training procedure and demonstrated that ANN can be made as reliable as current artificial intelligence symbolic

methods. A second type of ANN was added to the model to permit the network to learn from the experience of the decisions made during the operation of the computer simulation. The second ANN had the same architecture as the first ANN with the addition of a goal node and goal sub-nodes. The goal that was used in this example was to maximize the difference between the Orange losses and the Green losses. An unsupervised training algorithm was used to permit the network architecture to adapt to the information provided by additional replications of the computer simulation. An unsupervised training process does not require a teacher that knows what the outputs should be for the training inputs. This example demonstrates that artificial neural networks could be used to develop "adaptive simulations."[84]

A final application of ANN that is of relevance to this dissertation is the use of neural networks as c- -llers. Much work has been done using actual system data to develop neural network controllers on systems as diverse as robots, automobiles, aircraft, space stations and manufacturing plants.[85-87] One group of researchers used neural networks trained on computer simulations to develop heuristic rules for scheduling a flexible manufacturing system.[88] One conceptual paper by Wan and Cochran, without any experimental results, outlines an approach to develop a controller for a system using a simulation of the system and a neural network approximation to the simulation.[89]

2.3 Metamodels

A metamodel is a "model of a model."[90] Blanning first used the term to refer to models of decision models and discussed computer simulation decision models as examples where metamodels could be used to perform sensitivity analyses.[91,92] Earlier,

Meisel and Collins had used the term "repro-model" to refer to a model of a model and described repro-modeling as the "process of developing an approximation to, or condensation of, a complex (sometimes dynamic) computer-based model."[93] It appears that metamodel has superseded repro-model as the commonly used term for a model of a model. On the basis of thirty experiments, Friedman and Pressman demonstrated the usefulness and applicability of metamodels in simulation analysis.[94] Pratt and Mize discuss a methodology developed for using metamodel of simulations of manufacturing systems.[95] Yu and Popplewell provide a summary review of the research that has been done in the field of simulation metamodels.[96]

Some researchers define a metamodel as a "regression model of the actual simulation model."[97] While it is true that the most popular technique used in metamodeling simulations is linear regression, there are alternative ways of developing a model of a model. In particular, this dissertation explores the use of artificial neural networks as metamodels of computer simulations. Barton discusses the state-of-the-art in metamodeling and provides an excellent review of several alternative metamodeling methods. He suggests the following criteria which might prove useful in choosing from among competing metamodeling techniques:[3]

1. The ability to gain insight from the form of the metamodel.
2. The ability to capture the shape of arbitrary smooth functions based on observed values which may be perturbed by stochastic components with general distributions.
3. The ability to characterize the accuracy of fit through confidence intervals, etc.
4. The robustness of the prediction away from observed (x,y) pairs.
5. The ease of computation of the metamodel.
6. The numerical stability of the computations, and consequent robustness of predictions to small changes in the parameters defining the metamodel.
7. The existence of software for computing the metamodel, characterizing its fit, and using it for prediction.

It is assumed that the goal in metamodeling is to obtain a function f, that will transform model inputs, **X**, into model outputs, **Y**, with a certain amount of error, ε, as depicted in equation 2-2.

$$\mathbf{Y} = f(\mathbf{X}) + \varepsilon \tag{2-2}$$

While some work has been done with predicting multiple output measures of computer simulations,[98] the typical approach has been to develop separate metamodels for each element of the simulation output measure vector.[3] Thus, for the discussion in this section, equation 2-3 which has the output measure, y, and the error of the approximation, ε, as scalars, will be used, rather than equation 2-2 which has the output measure and error as vectors.

$$y = f(\mathbf{X}) + \varepsilon \tag{2-3}$$

2.3.1 Linear Regression

Due to the popularity of linear regression, many researchers have come to think of metamodels as "models of simulation models, which express the input-output relationship in the form of a regression equation."[99] Since linear regression is a sound, well established statistical method, there are many textbooks that have detailed derivations of the relevant equations and formulas. Only the basic elements of polynomial multiple linear regression are discussed here. The notation and the derivation of the regression equations found in this section are based on Draper and Smith.[100] In regression, there are two types of variables: the independent or predictor variables (**X**) and the dependent or response variable (y) that are related by the equation 2-3.

Suppose there are n observations of pairs $(\mathbf{x}_i, y_i)$ with m elements in each vector $\mathbf{x}_i$ and that there are k power functions $Z_j(\mathbf{x}_i)$ of the independent variables. For example, for a first-order regression equation, the power functions would be $Z_0(\mathbf{x}_i) = 1$, $Z_1(\mathbf{x}_i) = x_{i1}$, $Z_2(\mathbf{x}_i) = x_{i2}$, ..., $Z_m(\mathbf{x}_i) = x_{im}$. For higher order regression equations, the power functions might be $(x_{i1})^2$, $(x_{i1})^3$, or $(x_{i1})^2(x_{i2})$. The regression problem is to find the values of the coefficients β that provide the least squared error to the solution of the system of equations given in equation 2-4. The corresponding matrix form of the system of equations is given in equation 2-5, where Y is an (n x 1) column vector, Z is an (n x k) matrix, β is a (k x1) column vector and ε is an (n x 1) column vector. The regression solution to these equations is given in equation 2-6. It should be noted that the reason this is called linear regression is that the equation is linear, not in terms of the predictor variables, but in terms of coefficients of the equation. Also, it is called multiple regression because there is more than one independent variable.

$$y_i = \left(\sum_{p=1}^{k} \beta_p \times Z_p(\mathbf{x}_i) \right) + \varepsilon_i \quad \text{For } i = 1, 2, \ldots, n \tag{2-4}$$

$$\mathbf{Y} = \mathbf{Z}\beta + \varepsilon \tag{2-5}$$

$$\beta = (\mathbf{Z}'\,\mathbf{Z})^{-1}\mathbf{Z}'\,\mathbf{Y} \tag{2-6}$$

The standard assumptions made in regression are that the errors have a mean of zero and a common variance and that the errors are not correlated with each other. [101] The assumption that the errors will have a common variance is often invalid when approximating computer simulations. While not totally effective, weighted least

squares[102] or transformations of the dependent variable[103] are sometimes used when the assumption of common variance cannot be made. Additionally, a typical assumption is made that the errors are distributed normally with mean of zero and a common variance. This final assumption permits the construction of confidence intervals for the coefficients of the model as well as for the predictions of the model. In those cases where normality of errors cannot be assumed, an alternative approach is to use the generalized linear model which assumes that the errors come from any family of exponential distributions rather than restricting them to the normal distribution.

While there are many strengths of polynomial regression models, there are also some weaknesses. Low-order polynomials have a very limited number of surface shapes that can be approximated, while high order polynomials have the tendency for errors to increase rapidly as the independent variables are moved away from an observation used to build the regression model.[3]

The field of regression is continuing to grow and expand as evidenced by work in such areas as nonlinear regression[104,105] and nonparametric regression.[106,107]

2.3.2 Response Surface Methodology (RSM)

Using the term metamodel to mean a "model of a model" is relatively new. However, the most popular metamodel approach of using low-order linear regression models in response surface methods (RSM) was formally developed in 1951 by Box and Wilson to optimize the yield of chemical processes through a series of physical experiments.[108] Since then response surface methods have been extended to include using regression models to optimize computer simulations. The purpose of RSM is to find

the levels of the experimental factors that will yield the best value of the response or output of a system. The response surface methodology with computer simulation basically entails a repetitive process of performing the following steps:[109]

1. Conduct a set of designed experiments that finds the output response value by running the computer simulation at various levels of the input parameters for multiple replications.

2. Approximate the relationship between the input parameters and the output measures in the current region of interest with a model of the system. Typically, the approximating models have been first-order regression models.

3. Find a direction in the input parameter space of the model that yields improved solutions (e.g., in the direction of the gradient, if trying to maximize the response).

4. Move in the direction of improved response and return to Step 1. If there is no direction of improved response, then develop second-order regression models to obtain a more accurate characterization of the response surface. Use this second-order regression equation is to determine if the found region is a locally optimal.

For optimizing computer simulations with single output measures, first-order regression models are good tools for determining the direction of search in response surface methods because they can be developed very quickly and it is very easy to determine the direction of improvement once the model is developed. Although most of the work in RSM has been with optimizing one dimensional output measures, some work has been done on optimizing computer simulations with multiple output measures.[102] Improved results have been reported when using different variance reduction techniques

such as combining common random numbers and antithetic variates in response surface methods.[12,110,111]

A good approximation in RSM is needed only in a small region of interest since the regression models are constantly being replaced as the search for the optimum progresses across the input space. Hood and Welch provide an excellent description and example of using RSM with computer simulations.[112]

2.3.3 Taguchi Models

Just as with response surface methods, the Taguchi method was not originally developed to be used with computer simulations, but with physical systems.[113] Taguchi developed a very successful method of designing quality into products that was easier to understand and use by practicing engineers. The Taguchi method using direct physical experiments is well documented.[114,115] Recently, the Taguchi method has been successfully used in system design with computer simulation experiments.[116-119] At the core of Taguchi's method is the precept that rather than try to eliminate the sources of variability in product performance the focus should be on trying to develop products that are not sensitive to the effects of uncontrolled variation. The Taguchi method uses the same model as equation 2-4 and assumes the errors of the models have a mean of zero (i.e., $E(\varepsilon_i) = 0$). Instead of assuming that the variance of the errors is a constant however, it assumed that the variance depends on the value of the independent variables (i.e., $Var(\varepsilon_i) = \sigma^2(X_i)$). Taguchi incorporates the information about the variance of the system by introducing equation 2-7 where the $\overline{Y}$ is the sample average and the s^2 is the sample variance over the multiple observations at each combination of the independent variables.

$$10 * \log\left[E\left(\bar{y}^2 / s^2 \right) \right] = \sum_{p=1}^{k} \gamma_p \times Z_p(x) \qquad (2\text{-}7)$$

The other variables in equation 2-7 are described in the section on linear regression. Under Taguchi's approach, it is expected that some independent variables, **x**, will have small coefficients of γ_p in equation 2-7 and large coefficients of β in equation 2-5. Those independent variables with small coefficients of gamma are termed "insensitive to noise." By adjusting the remaining independent variables to maximize the left side of equation 2-7, the analyst can then set the independent variables to produce the desired minimimum or maximimum of the response in equation 2-5.[3,120] The Taguchi approach provides an alternative framework to traditional design of experiments and response surface methods, within which neural network metamodeling can be used.

2.3.4 Approximation Theory

This established field of mathematics is concerned with problems associated with approximating continuous, multivariate functions whose values are known at a finite number of points. This requires determining the values of a fixed number of parameters **W**, so that an approximating function, $F(\mathbf{X},\mathbf{W})$, provides the 'best' approximation or estimation to the desired function, $f(\mathbf{X})$.[121] Often the approximating function $F(\mathbf{X},\mathbf{W})$ is a linear combination of basis functions, $g_i(\mathbf{X})$, for example $F(\mathbf{X},\mathbf{W}) = \Sigma a_i \times g_i(\mathbf{X})$, where the a_i are real valued constants. This approach is used in many of the classical methods of approximating functions including polynomial approximation, spline approximation, kernel based approximation, and Fourier methods.[122] These and other classical methods suffer from the need to correctly specify the functional form of the model that will be used in the

approximation procedure. In most cases the correct functional form of the model depends on the data observed from the function. Also, many of the methods assume that the observed function values are correct (i.e., there is no noise in the data).

The computer simulations examined in this research are stochastic and so they are not strictly functions. Many of the simulations found in the industrial engineering literature are of systems with discrete, rather than continuous, input values. In addition, a linear combination of basis functions can be implemented efficiently via a three layer, artificial neural network, where each basis function is represented by a node in the hidden layer of the network.[123] For these reasons, the approaches used within the field of approximation theory were not explored further for application to approximating computer simulations.

2.4 Summary

This chapter provides a survey of the literature concerning the topics involved in this dissertation. The chapter contains discussion of the broad areas of computer simulation, metamodels and artificial neural networks each of which are relatively new fields of research beginning in the 1940s, 1960s and late 1980s, respectively. The history of each of these fields as well as the definitions of key terms and a review of the literature relevant to this research are covered. The field of computer simulation is shown to be quite wide in its scope and applicability to many diverse disciplines. The limitations of computer simulations for performing studies quickly, sensitivity analyses, and optimization of systems are delineated. The discussion of artificial neural networks includes a detailed exposition of the backpropagation training methodology and several examples of other

researchers using ANN in conjunction with computer simulations. The discussion of metamodels includes the history and terminology of metamodels, regression, response surface methodology and approximation theory.

3.0 RESEARCH METHODOLOGY, ISSUES AND TOOLS

3.1 Methodology of Research

The general research methodology of this dissertation is to develop an approach to approximating computer simulations using ANN. This is done in two stages. First, investigating issues through experimentation on a computer simulation of a relatively simple engineering system. The second stage is to demonstrate the approach on a computer simulation of a much more complex engineering system. Seven tasks were defined and are discussed below.

3.1.1 Basic Research Tasks

The first task was to identify the issues that need to be considered for any generic approach to approximating discrete event, stochastic computer simulations and the specific issues that might be unique to an artificial neural network (ANN) approach. A listing of the identified issues is provided in Section 3.2.

The second task was to obtain detailed computer simulation models of two real world systems that were representative of the types of problems typically examined using terminating, stochastic, discrete-event computer simulations in the field of industrial engineering. The first system examined was a relatively simple inventory system. This system was selected to be able to make comparisons to the problem used in Chapter 12, "Experimental Design and Optimization" by Law and Kelton.[124] This system was analyzed in-depth in order to gain insight into how to approximate a computer simulation with an ANN model. In this manner, the first system was used as a problem for

developing the methodology for approximating computer simulations with ANN. The description of the system and its computer simulation are presented in Chapter 4. The second system examined in this research was the emergency department of a large teaching hospital. This system is representative of large, complex systems and was used as a research demonstration problem to examine issues of "scale-up" and applicability of the methodology to "real world" problems. The description of the system and its computer simulation are presented in Chapter 7.

The third task was to develop, build, and use simplified representations of the development problem computer simulation model based on the ANN techniques. A series of experiments was performed on a two-input parameter version of the inventory system simulation. These experiments considered various ways of presenting the output of the simulations to the ANN and predicting multiple outputs. The detailed description and results of these experiments are also presented in Chapter 4.

The fourth task was to use the ANN approximations of the inventory system in place of the original computer simulation model to perform basic computer simulation tasks of prediction and comparison of alternatives. Part of this task was to compare the results of the ANN approximation to a second-order multiple linear regression model approximation. The second-order multiple linear regression model was used for comparison purposes since it is the highest order regression model typically used in Response Surface Methods. The final set of experiments used ANN approximations to make predictions and prediction intervals for the four input parameter inventory system simulation are discussed in Chapter 5.

The fifth task was to develop a methodology for approximating computer simulations with ANN, based on the results of the experiments on the development problem. The resulting approach is presented in Chapter 6.

The sixth task was to apply the approach of ANN approximation of computer simulations to the demonstration problem (i.e., emergency department system). The results of applying the ANN approximation approach to the demonstration problem are also provided in Chapter 7.

The final task was to synthesize the lessons learned from performing the basic simulation tasks with ANN approximations to computer simulations to provide a framework for using ANN approximations to perform more complex simulation tasks such as sensitivity analysis, simulation "optimization," and model aggregation/reduction. These results are discussed in Chapter 8.

3.1.2 Assumptions and Restrictions of the Research

Since the focus of this research effort was to develop a tool that could be used to approximate a computer simulation, it was assumed that the topology of the internal relationships and procedures within the computer simulation were determined and would not be modified (i.e., the computer simulation to be approximated has already been finalized, verified, and validated). Consequently, this research did not address problems associated with building computer simulation models. It was assumed that only the values of the input parameters that were provided to the computer simulation could be changed.

The prediction of output values was only done for those values determined at the end of the simulation. Predicting intermediate results of the output measures over time is a subject for future research efforts.

This research only examined terminating, stochastic, discrete-event computer simulations. A description of these terms is provided in Chapter 2. This research focused on the types of computer simulations typically used for addressing industrial engineering/management science/systems analysis problems. However, this same approach could be utilized and should be fruitful in other areas.

Feedforward, multi-layered, fully connected artificial neural networks trained via the backpropagation learning algorithm were used in this research. Specifically, the basic backpropagation method popularized by Rumelhart, Hinton and Williams[45] for training feedforward, fully connected ANN was used for the reasons specified in Chapter 2.

This research used a comprehensive, one-step, experimental design for selecting the points to be simulated and subsequently used for developing approximations to the computer simulation. An alternative approach, which was not used in this research, is sequential experimental design which incorporates information about the responses of the simulation from preliminary design points to guide the selection of subsequent design points. The sequential experimental design approach is typically preferred when conducting computer simulation sensitivity analysis and when using response surface methods.[125] The work in this research addresses how to do the comprehensive experimental design and the first step in the sequential experimental design.

3.2 Research Issues

The following research questions were identified for consideration and/or experimentation:

How should the simulation output data be presented to the ANN during training?

How many outputs should be predicted by a single network?

Can the ANN predict the descriptive statistics commonly used in computer simulations (e.g., mean, variance, minimum, maximum)?

What should the network architecture be for the ANN?

How many different combinations of the input parameters (i.e., experimental design points) should be used during training?

How many replications of the computer simulation of each combination of the input parameters should be used during training?

How well does the ANN approximation perform in making predictions of simulation output measures?

How well does the ANN approximation perform in making prediction intervals of simulation output measures?

How does an ANN approximation compare with second-order multiple regression approximations of computer simulations?

3.3 Research Tools

Two commercial products were used extensively in this research: SIMAN/CINEMA© and BrainMaker©. A description of each of these tools and a discussion as to why they were selected is provided below.

3.3.1 SIMAN/CINEMA Simulation Language

SIMAN/CINEMA has been developed by Systems Modeling Corporation of Sewickley, PA, as a general-purpose simulation modeling language with additional features that make it very useful for modeling manufacturing systems. The SIMAN (SIMulation ANalysis) portion of the package is used to create the actual simulation while the CINEMA portion is used to provide an animation of the simulation.[126]

A simulation language as opposed to a programming language such as FORTRAN or Pascal was chosen for use in this research since the majority of work in the simulation of industrial engineering applications uses higher-level simulation languages.

The SIMAN simulation language was chosen for use in this research for the following reasons. SIMAN was one of the first major simulation languages available for use on microcomputers, and it is used extensively in the industrial engineering and manufacturing fields.[126] SIMAN operates on a wide variety of computer platforms, and the programs are compatible across the different classes of computers. Hence, SIMAN is available to many researchers who might be interested in pursuing this research. It is possible to model almost any kind of system using SIMAN, due to its ability to utilize the two major approaches used in discrete-event simulation: the event-scheduling approach and the process interaction approach. SIMAN is relatively easy to use, and has a good debugging facility. Another reason for selecting SIMAN/CINEMA is the ability to use CINEMA to animate the simulation for the purpose of verifying and validating computer simulations. SIMAN also employs Zeigler's theoretical concepts about systems by placing the system information into two separate component frames of the simulation.[127] The physical elements of the system and their interconnections comprise a functional

description of the system in a "model" frame. The input parameters and the data associated with the conditions under which the simulation is to be conducted are placed in an "experiment" frame.[128] This feature greatly assists in performing research experiments by insuring that changes to the input parameters do not alter the processing steps of the simulation.

The SIMAN package used in this research was SIMAN IV with runtime processor version 1.3. The CINEMA package used in this research was CINEMA IV version 1.2. The simulations were all run on a 486/33mhz personal computer under DOS 5.0.

The SIMAN model and experiment frames for the research development problem (i.e., the inventory system) are contained in Appendices A and B, respectively.

3.3.2 BrainMaker Neural Network Computing Package

BrainMaker is a commercial software product from California Scientific Software of Nevada City, CA for backpropagation neural networks. Unlike some of the other commercially available products that permit a wide variety of different artificial neural network paradigms, the BrainMaker product has concentrated exclusively on the backpropagation method of training ANN. As a result, BrainMaker is a very flexible and widely accepted platform for use in performing research on artificial neural network issues and problems concerning backpropagation training of ANN. One of the major differences between standard backpropagation and BrainMaker's backpropagation, is that BrainMaker uses a smoothing factor (usually called momentum) to provide a means of performing exponential smoothing for the inputs used in training the ANN. Another difference is that BrainMaker only attempts to learn a particular training point if it is not within the pre-

specified tolerance of its intended target. The other major difference is that standard backpropagation only terminates when all of the training outputs are within the pre-specified tolerance of their targets. BrainMaker can also be instructed to terminate training when a pre-specified number of passes through the data have occurred.[129]

BrainMaker was selected for use in this research for the following reasons. First, it is a widely available and accepted product, so that other interested researchers can examine, verify and continue this research effort. BrainMaker has been extensively tested and has been found to correctly implement the backpropagation training algorithm. The graphical user interface for BrainMaker is very user-friendly. The ability to conduct training and testing in batch mode using DOS batch files also permits training hundreds of ANN in a systematic and efficient manner. BrainMaker has several flexible stopping criteria options: 1) either the MAE (Mean Absolute Error) tolerance on all or a pre-specified proportion of input vectors; 2) train until reaching a pre-specified number of presentations; 3) train and save. This last option permits postprocessing of the training results in order to find the best trained network. A final reason for using BrainMaker was the ability to automatically generate "C" code for the trained network for use in future optimization and direct integration with database and spreadsheet programs. The BrainMaker software package used in this dissertation was BrainMaker Professional version 2.53. All cases of training and testing using BrainMaker were performed on 386 and 486 personal computers under DOS 5.0.

The derivation of the backpropagation method of training is well documented in the literature and is not repeated here.[45,130,131] The essential elements of the

backpropagation method of training as implemented in the BrainMaker software used in this research are described here for a fully connected feedforward network.[132]

Initialization Step: All weights, w_{ij}, which is the weight of the connection going from node j to node i, are initialized to random values between -8.0 and 8.0. Training tolerance (Tol = 0.1), maximum training cycles (Max Cycles=99999), training rate or gradient step size (η = 1.0) and smoothing factor (μ = .9) are set, where the values in the parentheses indicate default values. Also to count the number of training cycles, an internal counter variable is initialized to zero (i.e., Training Cycles = 0). To determine how many training points have not been learned to the desired tolerance, a counting variable is set to zero (i.e., Number Bad = 0) The transfer function is selected with the logistic function given in equation 3-1 as the default with β = 1.0. The training and test data are scaled to the interval [0,1].

$$t(x) = \frac{1}{(1+e^{-\beta x})} \tag{3-1}$$

Step 1. Feed input vector values forward through the network one layer at a time from the input layer to the output layer to obtain activations at each node and the response vector values. A training point, (Ip, Tp), is selected from the training set of size P. The formulas for calculating the input layer, hidden layer, and output layer activations are given in equations 3-2, 3-3, and 3-4 respectively. Note that $R_i(p)$ is the response of the ith output node for the pth training point. The fan-in of a node includes all of the arcs that come into the node.

$$A_i(p) = I_i(p) \tag{3-2}$$

$$A_i(p) = t\left(\left(\sum_{j \in \left\{\begin{matrix}\text{fan-in} \\ \text{node } i\end{matrix}\right\}} w_{ij} \times A_j(p)\right) + w_{io} \times V_i\right) \tag{3-3}$$

$$R_i(p) = A_i(p) = t\left(\left(\sum_{j \in \left\{\begin{matrix}\text{fan-in} \\ \text{node } i\end{matrix}\right\}} w_{ij} \times A_j(p)\right) + w_{io} \times V_i\right) \tag{3-4}$$

Step 2. Compute the squared error, E(p), for training point p according to the formula given in equation 3-5 where J equals the number of output nodes.

$$E(p) = \frac{1}{2} \sum_{j=1}^{J} \left(T_{j(p)} - R_{j(p)}\right)^2 \tag{3-5}$$

If E(p) > Tol, then this pattern has not been learned to the desired tolerance level and the variable Number Bad is set equal to Number Bad + 1 and proceed to Step 3.

If E(p)≤ Tol, then this pattern was learned to the desired tolerance so go to Step 5.

Step 3. Calculate the error signals for all output and hidden nodes, beginning at the output layer and working backward through the network, one layer at a time. The error signals are calculated for the output nodes with equation 3-6 and for the hidden nodes with equation 3-7.

$$\delta_j(p) = R_j(p) \times (1 - R_j(p)) \times (T_j(p) - R_j(p)) \tag{3-6}$$

$$\delta_j(p) = A_j(p) \times (1 - A_j) \sum_{i \in \left\{ \begin{matrix} \text{fan-out} \\ \text{node } j \end{matrix} \right\}} (\delta_i(p) \times w_{ij}) \tag{3-7}$$

Step 4. Once all of the error signals for each of the hidden and output nodes are calculated in Step 3, the weights between each of the nodes are adjusted using the formulas in equations 3-8 and 3-9. If an exponential smoothing factor is used then equations 3-8 and 3-10 are used to adjust the weights. $\Delta w_{ij}(p)$ is defined as the change to the weight from node j to node i as a result of pattern p.

$$w_{ij} = w_{ij} + \Delta w_{ij}(p) \tag{3-8}$$

$$\Delta w_{ij}(p) = \eta \times \delta_i(p) \times A_j(p) \tag{3-9}$$

$$\Delta w_{ij}(p) = \eta \times \left[((1-\mu) \times \delta_i(p) \times A_j(p)) + (\mu \times \Delta w_{ij}(p-1)) \right] \tag{3-10}$$

Step 5. If $p < P$, then return to Step 1 and select the next training point. If $p = P$, then go to Step 6.

Step 6. Check the stopping criteria. If Number Bad = 0, then all training points have been learned to the desired training tolerance and so training should stop.
If Number Bad > 0, then at least one training point has not been learned to the training tolerance. Let Training Cycles = Training Cycles +1. If Training Cycles < Max Cycles,

then go to Step 1 and begin another training cycle with the first training point, otherwise stop.

The adjustment to the weights in Step 4 occurs as each training point is presented to the network in what is known as pattern training. To implement true gradient descent on the squared error surface would require the summation of the amount to change the weights for each of the training points with the actual change only being made at the end of each training cycle or epoch, in what is known as batch training. While BrainMaker has an option to perform training in this manner, it was not used in this research since it is more likely to become trapped in a local minimum of the error surface and it typically results in an increase in training time.(133)

3.4 Summary

This chapter provides an overview of the research issues and the methodology used to conduct the research in this dissertation. The research issues were developed and refined throughout the research effort. The methodology for conducting the research was to use an inventory computer simulation to perform a series of experiments in building ANN metamodels in order to develop a baseline ANN metamodel approach and to then demonstrate the use of the approach on a more complicated computer simulation, namely of an emergency department. Detailed discussion is included on the assumptions and restrictions of the research which are initially stated in Chapter 1. Specific details are provided on the two commercial software packages used to perform the research, SIMAN/CINEMA and BrainMaker. The SIMAN/CINEMA package was used to perform the stochastic computer simulations for the research problems. The BrainMaker package implements backpropagation training on feedforward artificial neural networks.

4.0 DEVELOPMENT PROBLEM - INITIAL EXPERIMENTS IN APPROXIMATING AN (s,S) INVENTORY SYSTEM

The approach taken in this research was to use a simple, yet realistic, model of a fairly complex engineering system as a testbed for various methods to approximate computer simulations using artificial neural networks. This chapter covers the initial experiments performed in approximating the computer simulation of an (s,S) inventory system with ANN. Using this particular system permitted the focus to be on developing the methodology of ANN approximation of computer simulations and not on computer simulation issues.

4.1 Description of the (s,S) Inventory System

The system used as a development problem in this dissertation was taken from Chapter 12 "Experimental Design and Optimization" by Law and Kelton.[134] The system is a probabilistic lot size-reorder point system, an (s,S) inventory system where s = reorder point quantity, and S = order up to quantity, with a time horizon of 120 months. It is difficult to obtain optimal solutions for these types of systems.[135] While progress has been made in developing algorithms for determining optimal policies of certain infinite time horizon versions of the (s, S) inventory problems, computer simulation is still necessary for examining many of the possible variants of the (s, S) inventory problem.[136] Law and Kelton constructed a series of first- and second- order regression model approximations, or metamodels, of a computer simulation of the inventory system. By increasing the number of data points, they were able to demonstrate that the metamodels could provide increasingly accurate approximations of the computer simulation.

The inventory system is representative of companies that sell a single product, with the problem of deciding how many items to obtain from their supplier in each of the next n *months in order to minimize the total cost of the inventory system.* There are several input and output parameters associated with this system. The input parameters of the simulation of the system include the following:

s = reorder point,

S = order up to quantity,

I = inventory level,

Z = reorder quantity,

d = S-s = reorder quantity when I = s,

D = size of demands,

t_d = time between demands,

t_o = time between order decisions,

t_L = time lag for delivery,

k = setup cost,

i = incremental cost per item ordered,

h = holding cost,

u = underage cost (cost of having to backlog orders),

n = time horizon for analysis purposes.

In Law and Kelton's sample problem, the parameters s and d were the only parameters that were treated as decision variables. The remaining input parameters were treated as uncontrollable factors and were assumed to be fixed at constant values. The following section describes the settings used for these uncontrollable factors, in Law and Kelton and in this dissertation.

The initial inventory level was set at $I_0 = 60$. In this system it is assumed that the company receives demands for its products on a periodic basis with the time between demands, t_d, distributed exponential with a mean of 0.1 month. The size of each demand, D is distributed according to equation 4-1.

$$D = \begin{cases} 1 & \text{with probability } \frac{1}{6} \\ 2 & \text{with probability } \frac{1}{3} \\ 3 & \text{with probability } \frac{1}{3} \\ 4 & \text{with probability } \frac{1}{6} \end{cases} \tag{4-1}$$

The time between order decisions, t_0, is one month. A stationary (s,S) policy is used to decide how much to order at the beginning of each month. In other words, given that I is the inventory at the beginning of the month, then the amount to order for that month, Z, is determined by equation 4-2.

$$Z = \begin{cases} S - I & \text{if } I < s \\ 0 & \text{if } I \geq s \end{cases} \tag{4-2}$$

In this system, the company determines each month whether or not it should place an order, and if so, how much to order. If an order is placed, then the time it takes for the order to arrive at the company, t_L, is distributed uniformly between 0.5 and 1 month. The total order cost is equal to $k + iZ$. In this problem $k = \$32$ and $i = \$3$. The holding cost per item per month held in inventory is given as $h = \$1$. The underage cost is given as $u = \$5$ per item per month in backlog (i.e., on order). The underage costs include such items as extra bookkeeping costs and loss of goodwill costs. The planning horizon or time that the system would operate under the various strategies of operating the inventory system was set at $n = 120$ months.

Some of the relevant output measures that could be calculated for this system, over the planning horizon, include:

Average total cost (C),

Average ordering cost,

Average holding cost,

Average shortage cost,

Average inventory level,

Minimum inventory level,

Maximum inventory level.

Law and Kelton used the computer simulation of the inventory system to obtain estimates of the output measure, average total cost per month (C) for various settings of the decision variables s and d. Since Law and Kelton used the inventory system to discuss the process of experimental design, they labeled the average total cost as R (for response of the computer simulation).

4.2 Computer Simulation of the Inventory System

The inventory system computer simulation used in this dissertation was written in the SIMAN simulation language for the reasons discussed in Chapter 3. Output statistics of different input parameter settings from a computer simulation can be categorized as either independent or dependent observations. In simulation, independent observations have been used quite widely due to the applicability of straightforward statistical tests for comparing alternatives. Dependent observations have been used for the purpose of variance reduction. One frequently used technique for producing dependent observations

is the common random number approach, one component of which is to use the same starting point in the same random number streams for each input parameter setting in a simulation run. Using the common random number approach would probably provide a more stable, but less robust, set of observations from the computer simulation since the variance is typically reduced. However, this research examined only the independent observations approach. One way that independent observations are obtained is to select different starting points in the same random number streams for each input parameter setting. In this research, independent observations for each input parameter setting were obtained by selecting the random number streams and running the simulation program through all of the desired replications by having the computer simulation iteratively read the input parameter settings from an external file. In this way the random number stream was never reset to the original starting point and thus created independent observations for all the replications of all of the input parameter settings. In some cases, due to memory restrictions of the computer, additional replications were made using different random number streams in order to preserve independence between the replications made for each input parameter setting. The same procedure was followed for all of the experiments performed in this research. For illustrative purposes the SIMAN computer programs and external data files that were used to produce the independent observations for this section are provided in Appendix A in Figures A1 through A3.

Validation of the SIMAN computer simulation was performed by comparing the output from the SIMAN simulation to the results given by Law and Kelton. Since Law and Kelton only provided the output of single simulation replications, a direct statistical comparison of the two is not possible. However, Law and Kelton did report the results of building first-and second-order regression models on multiple replications for different

input parameter settings. The approach used to validate the SIMAN simulation model of the inventory system was to build the same first- and second-order regression models on the SIMAN simulation data and compare the regression results to those found in Law and Kelton.

The two sets of input parameters given in Table 1 were simulated and used to build regression models. Each parameter setting consisted of a different combination of values of the input parameters s and d. The output measure of system performance, that was provided by the simulation, was the 120 month average, of monthly total cost, C. The SIMAN simulation results, where $\overline{C}$ is the average of C over ten replications, as well as the two input parameter settings for data sets A and B, are provided in Table 1.

Table 2 shows the regression models that were used by Law and Kelton to develop metamodels of the computer simulation. The Law and Kelton and SIMAN simulation results of ten replications of data set A, the first four input parameter settings from Table 1, were approximated using the first-order multiple linear regression model given in Table 2. The second-order multiple linear regression model in Table 2 was used to model the simulation results of five replications (from Law and Kelton) and ten replications (from SIMAN) of data set B, the second set of 36 input parameter settings from Table 1. It is not clear why Law and Kelton used only five replications at the 36 input parameters when all of the rest of their examples used ten replications. To maintain consistency between the models of the two data sets, ten replications were used in this dissertation for each model. The regression model results for the SIMAN data for data sets A and B are provided in Tables 3 and 4, respectively.

Table 1 SIMAN Simulation Results for Data Sets A and B

	s reorder point	d order quantity	$\overline{C}$ Cost				
Data Set A	20	10	136.56				
	20	50	120.81				
	60	10	145.20				
	60	50	149.01				
	s reorder point	**d order quantity**	**$\overline{C}$ Cost**		**s reorder point**	**d order quantity**	**$\overline{C}$ Cost**
Data Set B	0	5	233.17		60	5	140.34
	0	20	175.69		60	20	144.49
	0	40	147.69		60	40	145.52
	0	60	137.36		60	60	151.42
	0	80	134.14		60	80	158.92
	0	100	136.28		60	100	167.97
	20	5	147.41		80	5	161.40
	20	20	124.25		80	20	163.70
	20	40	119.73		80	40	165.50
	20	60	122.65		80	60	172.46
	20	80	127.06		80	80	179.13
	20	100	135.84		80	100	188.19
	40	5	127.13		100	5	181.54
	40	20	127.02		100	20	184.18
	40	40	126.49		100	40	185.19
	40	60	131.86		100	60	191.47
	40	80	140.30		100	80	200.84
	40	100	148.64		100	100	207.93

Table 2 Regression Models Used For Each Data Set

DATA SET	REGRESSION MODEL
A	$\text{Cost} = b_0 + b_1*s + b_2*d + \text{error}$
B	$\text{Cost} = b_0 + b_1*s + b_2*d + b_{12}*s*d + b_{11}*s^2 + b_{22}*d^2 + \text{error}$

Table 3 Regression for Data Set A Using SIMAN Simulation Results

Multiple R Square	0.89					
R Square	0.80					
Adjusted R Square	0.39					
Standard Error	9.78					
Observations	4					
	df	**Sum of Squares**	**Mean Square**	**F**	**P-Value**	
Regression	2	375.10	187.55	1.96	0.45	
Residual	1	95.73	95.73			
Total	3	470.83				
	Coefficients	**Standard Error**	**t Statistic**	**P-value**	**Lower 95%**	**Upper 95%**
Intercept	123.95	13.17	9.41	0.00	-43.42	291.31
s	0.46	0.24	1.88	0.16	-2.65	3.57
d	-0.15	0.24	-0.61	0.58	-3.26	2.96

Table 4 Regression for Data Set B Using SIMAN Simulation Results

Multiple R Square	0.88					
R Square	0.78					
Adjusted R Square	0.75					
Standard Error	13.94					
Observations	36					
	df	**Sum of Squares**	**Mean Square**	**F**	**P-Value**	
Regression	5	20916.50	4183.30	21.535	4.15E-09	
Residual	30	5827.49	194.25			
Total	35	26743.99				
	Coefficients	**Standard Error**	**t Statistic**	**P-value**	**Lower 95%**	**Upper 95%**
Intercept	189.40	9.22	20.54	4.15E-21	170.57	208.23
s	-1.51	0.26	-5.72	1.83E-06	-2.05	-0.97
d	-1.18	0.30	-3.95	0.0003	-1.79	-0.57
sd	0.010	0.00	4.80	2.91E-05	0.005	0.014
s^2	0.014	0.00	6.17	4.65E-07	0.010	0.019
d^2	0.007	0.00	2.59	0.0141	0.001	0.012

As can be seen from Tables 3 and 4 both models have approximately the same multiple R square values. The regression models in Tables 3 and 4 were built using the averages of the 10 replications at each data point. The same results in terms of the model coefficients result if the individual replications are used instead of the averages. However, in the regression model built on individual replications, the apparent goodness of the model increases due to a more significant F statistic caused by an increase in the degrees of freedom. In summary, the models provided by regression are the same for both averages and individual replications.

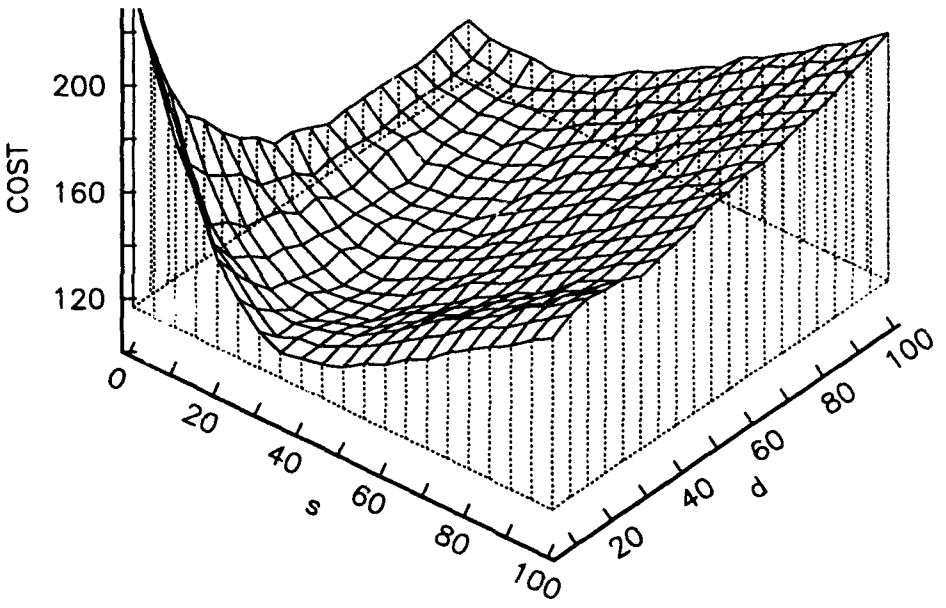
TABLE 5 Estimates of Regression Model Coefficients

DATA SET	SIMULATION DATA	REGRESSION MODEL
A	SIMAN	Cost = 123.95+0.46s-0.15d
A	LAW & KELTON	Cost = 125.37+0.44s-0.22d
B	SIMAN	Cost = 189.40-1.51s-1.18d+.010sd+.014s^2+.007d^2
B	LAW & KELTON	Cost = 188.51-1.49s-1.24d+.010sd+.014s^2+.007d^2

A summary of the regression results for each model in Table 2 is provided in Table 5 for both SIMAN and Law and Kelton simulation data.[137] There is close agreement in the coefficients of the regression equations for the SIMAN simulation data and the Law and Kelton simulation data for both data sets A and B. As can be seen from Tables 3 and 4, the 95% confidence intervals for each of the regression coefficients of the SIMAN data contain the regression coefficients obtained by Law and Kelton. Thus, for a Type 1 error of $\alpha = 0.05$, we do not have enough evidence to reject the null hypothesis that the SIMAN and Law and Kelton regression models are the same. This indicates that the SIMAN computer simulation models used in this research provide results that are similar to those produced by the computer simulations developed by Law and Kelton.

It should be noted that the last three values in the equation for Law and Kelton for data set B in Table 5 are mislabeled in the Law and Kelton textbook.[134] This can be seen by solving for the minimum of the function. The minimum value for the function in the textbook is found at s = 148 and d = - 42. By making the changes found in the table, in row D*, the minimum value is found at s = 29 and d= 68. These changes are also consistent with the contour diagrams of the function found in textbook and in Figure 9a discussed below.

Figure 9 shows three surface and contour plots of the space formed by s, d and cost as determined by direct simulation, a regression metamodel and an ANN metamodel. Figure 9a shows the surface plot and a contour plot of 420 equally spaced points on the (s,d) grid with the height of the surface and the contour lines representing the cost for each combination of s and d as determined by ten replications of direct simulation. This is basically the target that the metamodels are attempting to approximate. The regression model approximation to the target from Table 5, which was built on the 36 data points of set B, is shown in Figure 9b. As can be seen in Figure 9b, the model is smoother and has values that are too low in the lower left hand corner and values that are too high in the upper right hand corner. An artificial neural network approximation built on the same 36 data points of set B, is shown in Figure 9c. Visually, it appears that the ANN metamodel captures the essence of the surface better than the regression metamodel. In addition, the mean absolute error of the ANN evaluated at all 420 test points is 3.20 while the MAE is 8.64 for the regression model.[138]



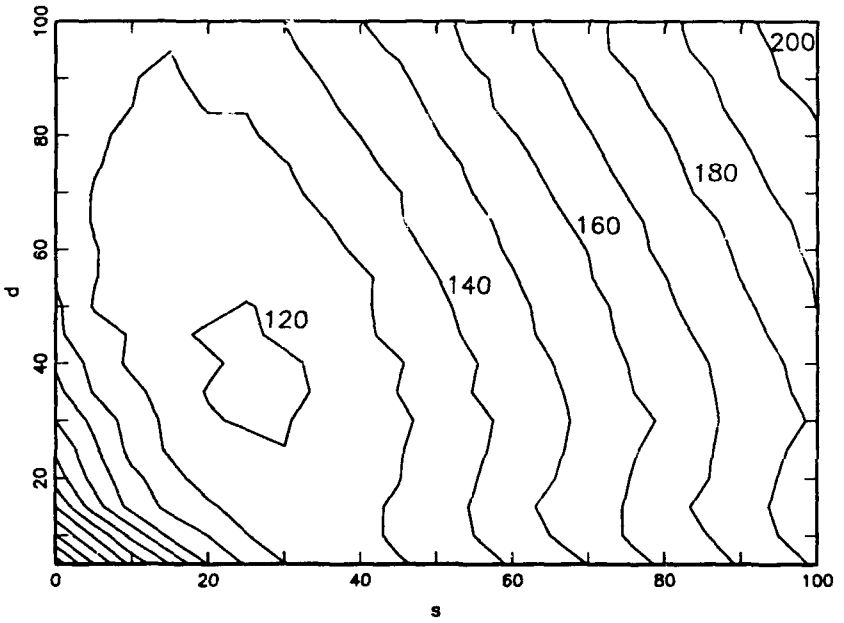
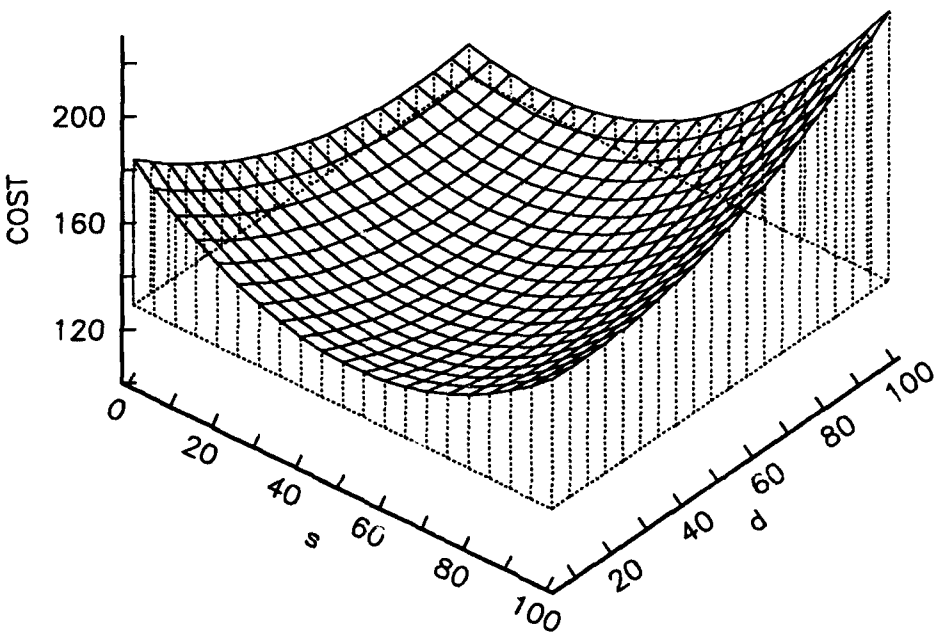


Figure 9a Direct Simulation at 420 Points



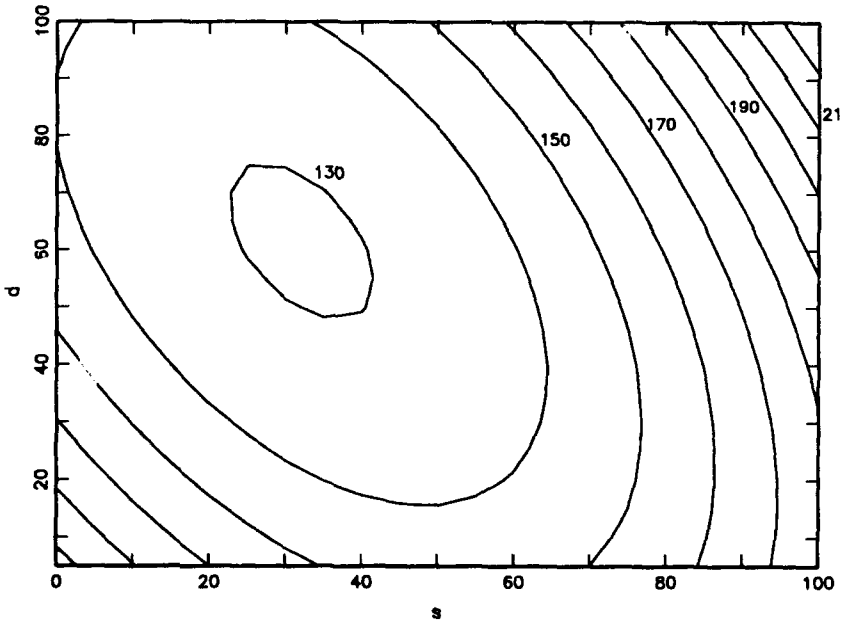


Figure 9b Regression Based on 36 Points

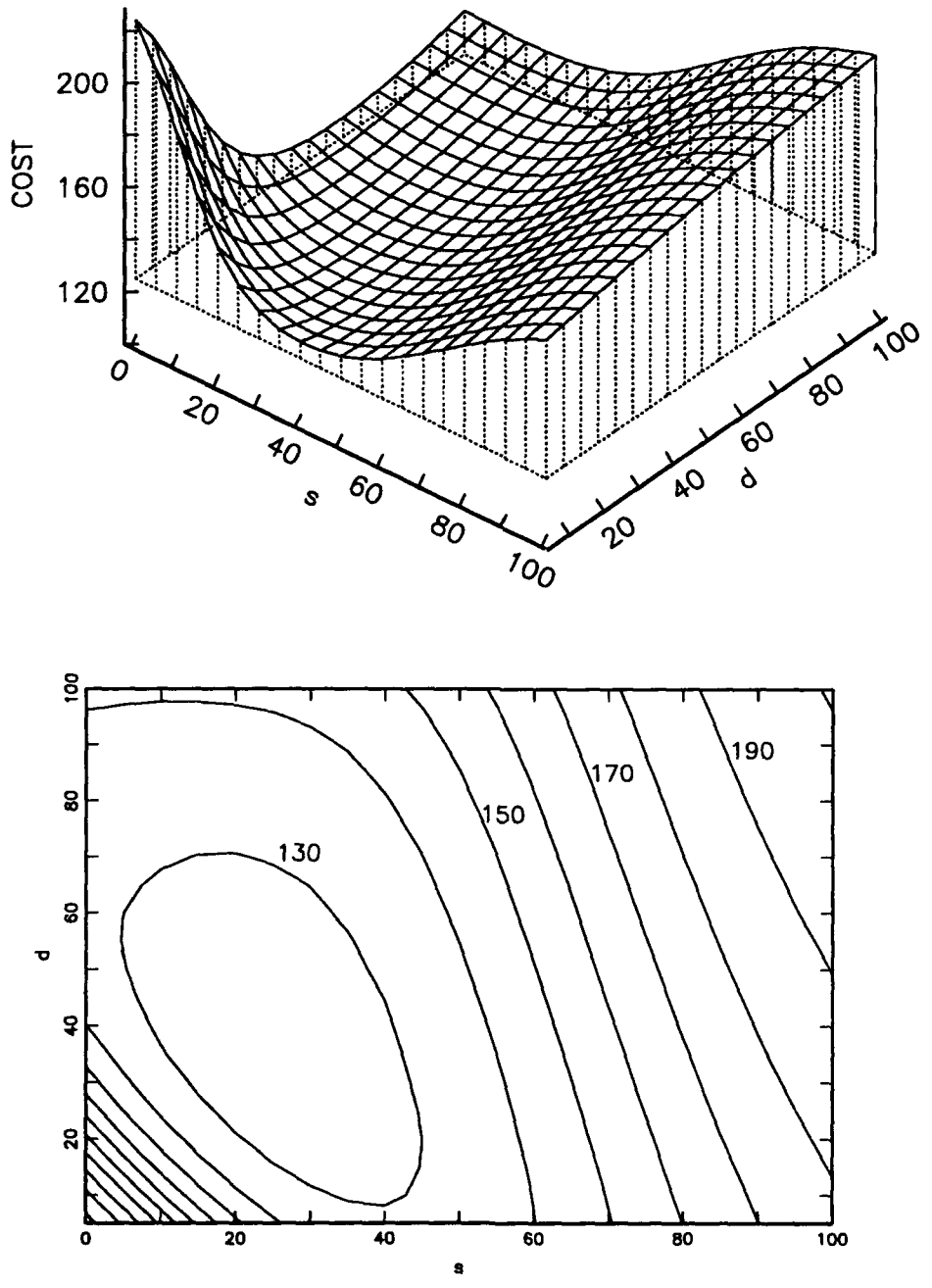


Figure 9c ANN Based on 36 Points

4.3 Experiments with Two Simulation Input Parameters

This set of experiments consisted of two different experiments. The first experiment consisted of predicting a single simulation output, mean cost. The second experiment predicted four typical descriptive statistics produced by computer simulations (i.e., mean, standard deviation, minimum, maximum).

The simulation of each input parameter setting consisted of operating the inventory system for a period of 120 months, or ten years of simulated time. The statistics used in these two experiments are calculated on the basis of the 120 months of operating the inventory system within each replication. Thus, at the end of each replication over the 120 months there is a minimum cost month, a maximum cost month and it is possible to calculate the average monthly cost and the standard deviation of the monthly costs. Finally, for each input parameter setting, multiple replications are performed and each of the relevant statistics are captured for each replication.

The purpose of these experiments is to examine the manner and the amount of simulation data to use in training an ANN to predict typical computer simulation outcome measures. One obvious way was to use just the average output values of the computer simulation replications at each input parameter setting. This seemed to eliminate information that the ANN might be able to take advantage of in building a better model of the computer simulation. Thus, the opposite extreme of using all of the simulation replications was also considered. Preliminary experiments showed that unlike regression, ANN metamodels built using averaged replication data performed differently than ANN built on individual replications. Concern about the effect of extreme points in the simulation data led to consideration of additional methods which used only the fifty

percent of the data that was nearest to the mean value. Finally, combinations of using averages and replications were also considered.

Specifically, five different methods of presenting simulation data to ANN were examined. The methods ranged from presenting all the individual replications to just the averages of the replications. The five presentation methods were:

Presentation Method 1 - Average output of all simulation replications.

Presentation Method 2 - All simulation replications and the average of all simulation replications.

Presentation Method 3 - Half of the simulation replications nearest to the average and the average of all simulation replications.

Presentation Method 4 - All simulation replications.

Presentation Method 5 - Half of the simulation replications nearest the average.

For each presentation method, the effect of increasing the number of simulation replications was examined. The number of replications of the computer simulation used for each input parameter setting was n = 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 15, 20, and 25.

The input parameter settings that were used to obtain data from the computer simulation to train the ANN for these experiments are shown in Table 6. As can be seen from Table 6, only two input parameters were allowed to vary: s and d. For illustrative purposes, the results of the computer simulation for each of the combinations of the input parameters shown in Table 6 for Experiment 1 and Experiment 2 for the average of 25 replications are provided in Appendix A, Table A1 and Table A2, respectively.

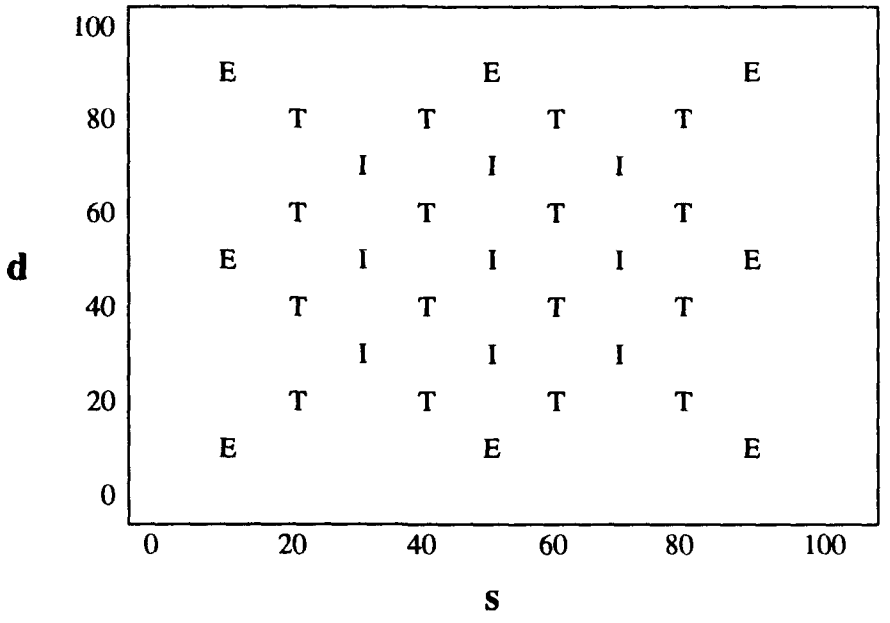
Table 6 Training Input Parameter Settings for Experiments 1 and 2

Input Parameter	Combinations of Training Input Parameter Settings							
s	20	40	60	80	20	40	60	80
d	20	20	20	20	40	40	40	40
s	20	40	60	80	20	40	60	80
d	60	60	60	60	80	80	80	80

The data used to test the ANN was obtained by running the computer simulation at the input parameter settings shown in Table 7. The test data was used to examine the ability of the ANN to generalize to previously unseen examples. The test set consisted of points that were completely internal to the training set and points that were completely external to the training set. The third grouping that was evaluated was the combination of all of the internal and external points. It was assumed that the average of the outputs of 500 replications for each input parameter setting of the test set from the computer simulation were the "right" answers. The metric for comparison purposes was the mean absolute error (MAE) of the difference between the outputs of the ANN and the computer simulations "right" answers. The test set "right" answers are provided in Appendix A, Tables A3 and A4, for experiments 1 and 2 respectively. A graphical portrayal of the location of the various training and test sets is given in Figure 10.

Table 7 Testing Input Parameter Settings for Experiments 1 and 2

Data Set	Input Parameter	Combinations of Testing Input Parameter Settings								
Internal	**s**	30	50	70	30	50	70	30	50	70
9 points	**d**	30	30	30	50	50	50	70	70	70
External	**s**	10	50	90	10	90	10	50	90	
8 points	**d**	10	10	10	50	50	90	90	90	



Input Parameters	Training & Testing points
s= Reorder point	T= Training points
d= Reorder quantity	I= Internal test points
	E= External test points

Figure 10 Training and Testing Points for Experiments 1 and 2

4.3.1 Experiment #1: Presentation Methods of Output Measures

The purpose of this experiment was to determine if there was a preferred way of presenting the replications of the computer simulation output measures as training data to ANN whose purpose was to predict a single simulation output. The SIMAN computer simulation of the system described in Section 4.2 was approximated by an ANN model using five different methods of presenting the training data. The five methods of presenting the computer simulation output data, C the average monthly cost, during the training of the ANN are shown in Table 8. The average cost over n replications used in

presentation methods 1, 2 and 3 is defined in equation 4-3.

$$\overline{C}_{j,k} = \frac{\sum_{i=1}^{n} C_{j,k}(i)}{n} \qquad (4\text{-}3)$$

Table 8 Methods of Presenting Simulation Output Data to ANN (Training Data)

Presentation Method	Input:	Output:
PM 1	s_j, d_k	$\overline{C}_{j,k}$ averaged over n replications
PM 2	s_j, d_k	$\overline{C}_{j,k}$ averaged over n replications & $C_{j,k}(i)$ for each replication, i.
PM 3	s_j, d_k	$\overline{C}_{j,k}$ averaged over n replications & $C_{j,k}(i)$ for the n/2 nearest replications to $\overline{C}_{j,k}$
PM 4	s_j, d_k	$C_{j,k}(i)$ for each replication, i.
PM 5	s_j, d_k	$C_{j,k}(i)$ for the n/2 nearest replications to $\overline{C}_{j,k}$
s_j, d_k represents a specific input parameter setting. n varied from 1 up to 25.		

For this experiment, a total of 59 distinct ANN were trained, 13 for presentation method 4, 12 for presentation methods 1 and 2, and 11 for presentation methods 3 and 5. However, the tables and figures showing the results for experiment 1 show 13 ANN for each presentation method, for a total of 65 ANN. The reason is that when the number of replications is only one, then the average is the same as individual replications and thus the

network for one replication from presentation method 4 was used as the network for one replication for all five of the presentation methods. Similarly the network for two replications from presentation method 4 was also used as the network for two replications for presentation methods 3 and 5.

All networks were fully connected and were constructed with two input nodes, two hidden layers with two nodes each, and one output node as shown in Figure 11. The learning rate was 1.0 and the smoothing factor was 0.9. Training continued until the network deemed a response as correct to within a training tolerance of 0.1 or 5000 passes through the entire data set. See Figures A4 and A5.

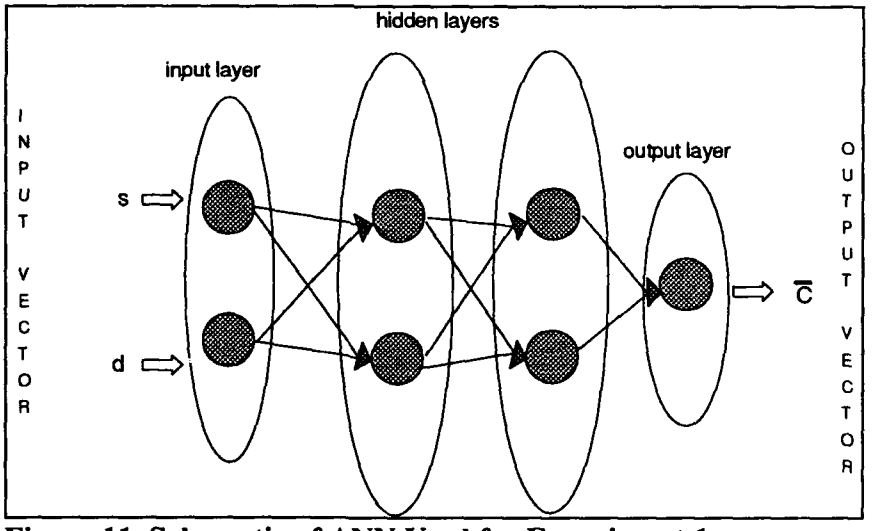


Figure 11 Schematic of ANN Used for Experiment 1

All of the ANN converged to the training tolerance of 0.1 for all of the presentation methods in experiment 1. The results of experiment 1 are summarized in Appendix A, Table A7. Figures 12 through 15 are based on the information provided in Table A7.

Figure 12 shows the results of evaluating the trained ANN on the training set. As can be seen from Figure 12 the values of MAE for the training set fall between 5 and 10. It appears that adding additional replications only improves the performance of presentation methods 2 and 4 when the training tolerance is fixed at a specified level.

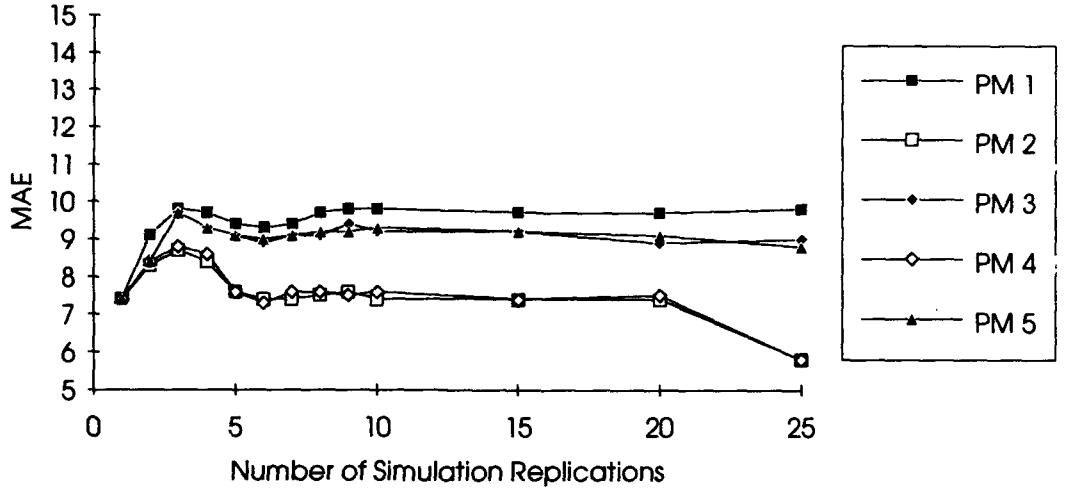


Figure 12 Training Set Results for Experiment 1

As can be seen in Figure 13 there is a cost associated with the improvement in the MAE for the networks trained using presentation methods 2 and 4. The cost is the increase in the number of presentations, or time required for the backpropagation algorithm to terminate the training process.

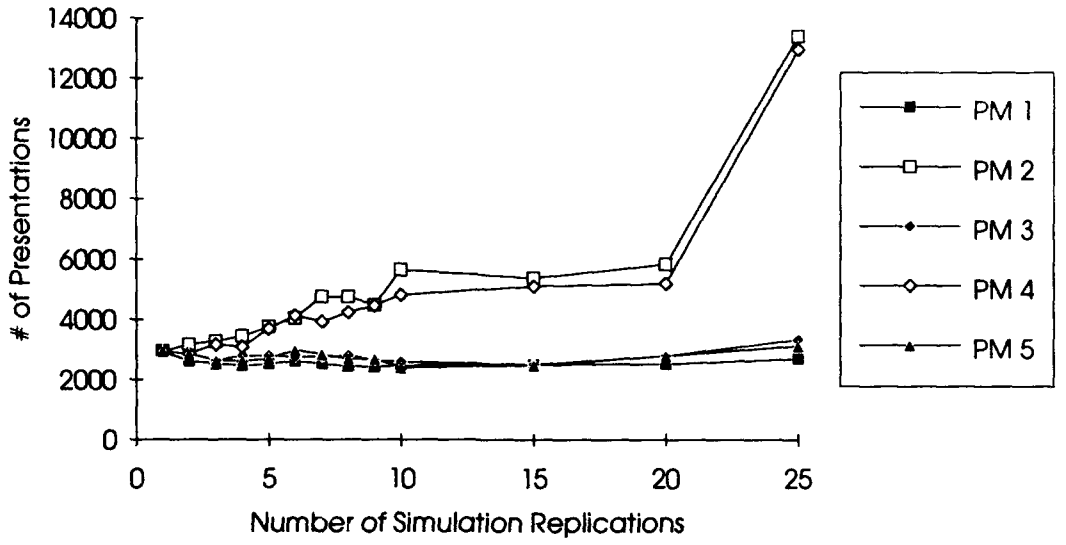


Figure 13 Presentations Required to Terminate Training for Experiment 1

The next group of charts, Figures 14 through 16, show the benefit of increasing the number of replications that are used for each training point on the ability of the trained ANN to perform on the test set. These figures show the results of testing each of the networks trained with the 5 different presentation methods. Figure 14 shows the results of the internal test set, Figure 15 shows the results of the external test set and Figure 16 shows the results of the combined test set. As can be seen in Figure 14, the ANN performance on the internal test set is between 5 and 10 MAE and from Figure 15, the results on the external test set are between 11 and 14 MAE. Obviously, and expectedly, the ANN are able to predict the computer simulation output values better for points that are internal to the training set rather than external to the training set. Thus we can say that ANN perform better as interpolating mechanisms rather than extrapolating mechanisms. The ANN performance on the combined test set ranges between 8 and 12 as can be seen in Figure 16. All three of the Figures 14, 15, and 16, indicate that presentation methods 2 and 4 do better than presentation methods 3 and 5 which did better than presentation

method 1. The conclusion from this experiment is that for a fixed value of the training tolerance with all networks converging to that training tolerance, it is better to use all of the replications of the data (presentation methods 2 through 5) rather than just the averages (i.e., presentation method 1). An additional conclusion is that ANN should be used with caution when performing extrapolations beyond the data on which they were trained. It also appears that there is very little difference between presentation methods 2 and 4 or between presentation methods 3 and 5. Thus from this experiment it appears that including the average along with the individual replications provides very little difference in learning the relationship between the inputs and outputs of the computer simulation.

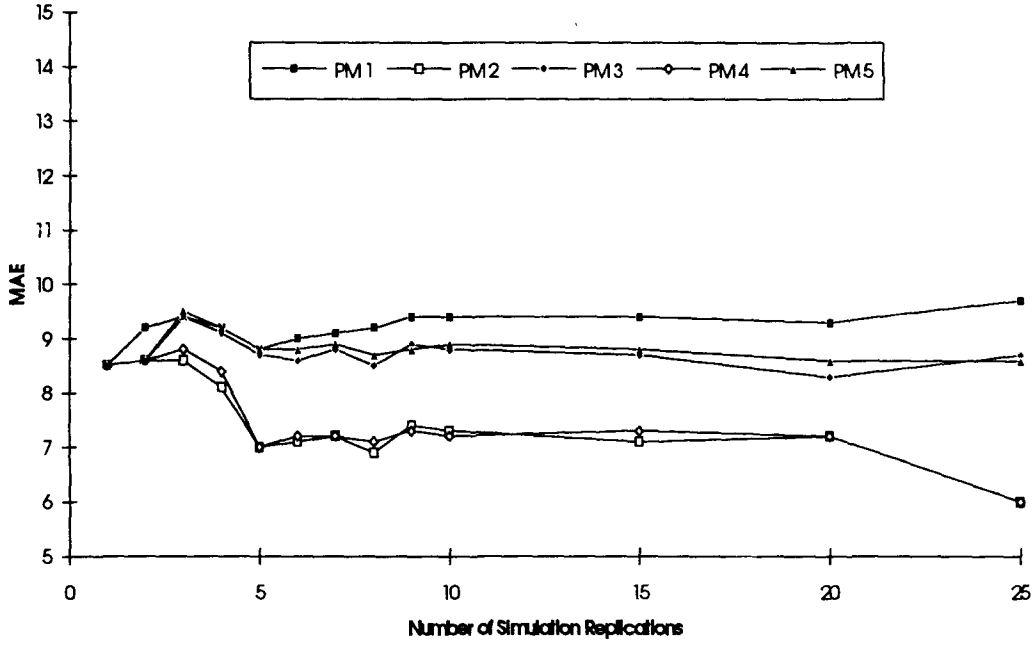


Figure 14 Internal Test Set Results for Experiment 1

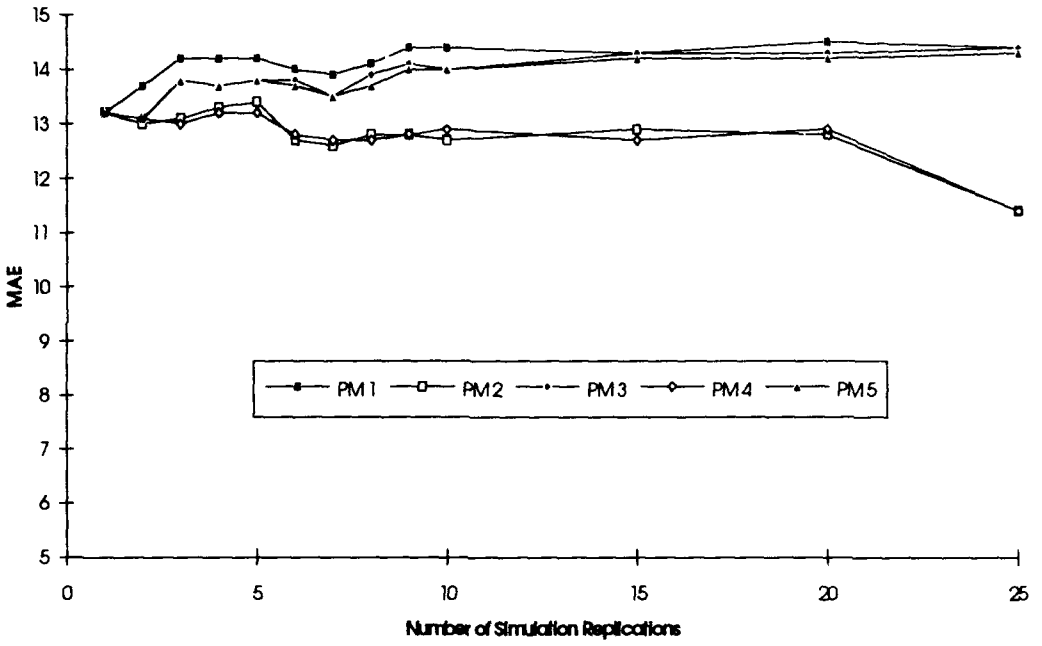


Figure 15 External Test Set Results for Experiment 1

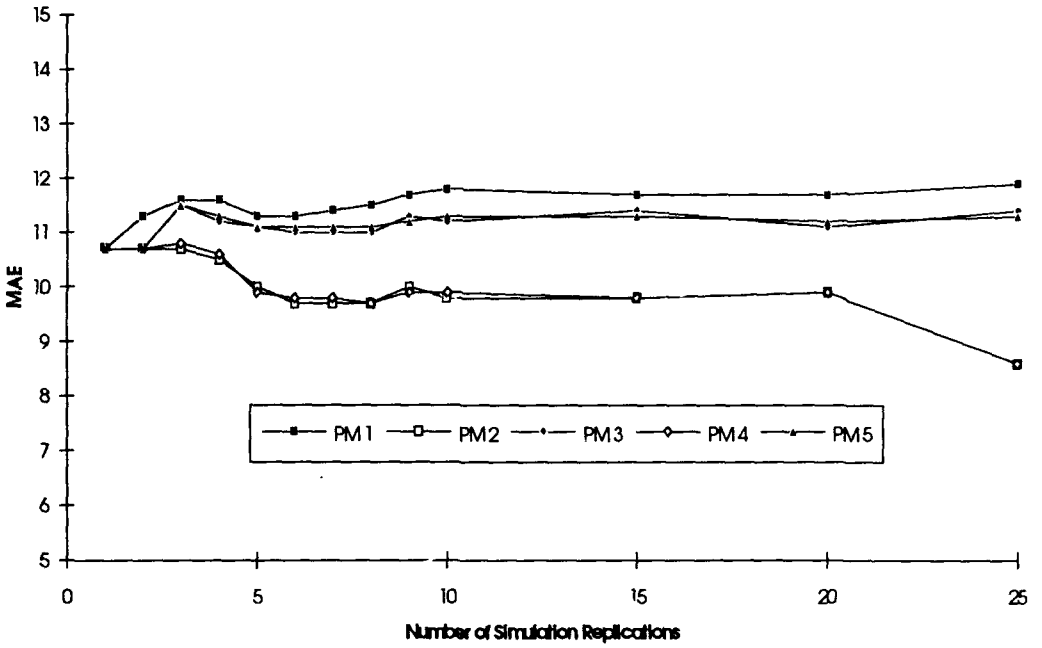


Figure 16 Combined Test Set Results for Experiment 1

4.3.2 Experiment #2: Predicting Descriptive Statistics Typically Produced by Computer Simulations (Mean, Standard Deviation, Min and Max)

The major difference between experiment 1 and experiment 2 is that experiment 2 used the ANN to predict three additional aspects of the desired measure of effectiveness. Both experiment 1 and 2 predict the mean value of the cost of operating the inventory system for 120 months. Experiment 2 also predicted the standard deviation, minimum and the maximum value of the cost for the same time period. These measures of cost are typical outputs provided by most computer simulation packages as the output of a single replication of the simulation. An example of the training data used for experiment 2 is the averages (i.e., presentation method 1) of the four different aspects of cost for 25 replications which is given in Table A2 of appendix A. The distinction between the internal, external and combined test points was examined in experiment 1 but was not considered in experiment 2. The only test set examined in experiment 2 was the combined test set which is provided in Table A4 in Appendix A.

For this experiment, a total of 59 different ANN were developed. All networks were fully connected and were constructed with two input nodes, two hidden layers with ten nodes each, and four output nodes. These networks have five times as many hidden nodes as were used in experiment 1, because it is a much harder problem to learn four outputs than to learn one output. Initial trials with a varying number of hidden nodes in each hidden layer yielded 10 hidden nodes per layer as a good starting point for this particular problem. Each input node corresponded to one of the input parameters (s, d), and each output node corresponded to one of the output parameters (mean, standard deviation, minimum, maximum). The learning rate was 1.0 and the smoothing factor was 0.9. Training continued until the network deemed a response as correct to within a

training tolerance of 0.1 for each of the four outputs or 5000 passes through the entire data set (See Figures A6 and A7).

The only presentation method to have all of the networks converge to the training tolerance of 0.1 for experiment 2 was the first presentation method. The results of experiment 2 are summarized in Appendix A, Table A8 for the training sets and Table A9 for the test set. The charts in Figures 17 through 25 are based on the information provided in Tables A8 and A9. The results in Tables A8 and A9 suggest, as was seen in experiment 1, that there is very little difference between presentation methods 2 and 4 or between presentation methods 3 and 5. Therefore, the figures showing the results for experiment 2 do not include presentation methods 4 and 5.

The results of the network evaluations of the training set for the various number of simulation replications for presentation methods one, two and three for the mean, standard deviation, minimum value, and maximum value of cost are shown in Figures 17, 18, 19 and 20, respectively. From these graphs it appears that there is some interference taking place between the various output measures that the neural networks are trying to learn. It appears from the fairly random nature of the Mean Absolute Error (MAE) for mean cost and minimum value of cost as seen in Figures 17 and 19 that this experiment has produced ANN that are not very consistent even for very small changes in the number of replications used to develop the ANN. This erratic behavior occurs for all of the presentation methods including the converging presentation method 1. The MAE for the outputs of standard deviation of cost and maximum value of cost as shown in Figures 18 and 20 are much more stable. An examination of the root mean square error (RMSE) for these measures in Table A7 and A8 in Appendix A, show that RMSE is much larger than MAE for the

standard deviation and maximum value of cost. This indicates that some of the errors are very large for these measures.

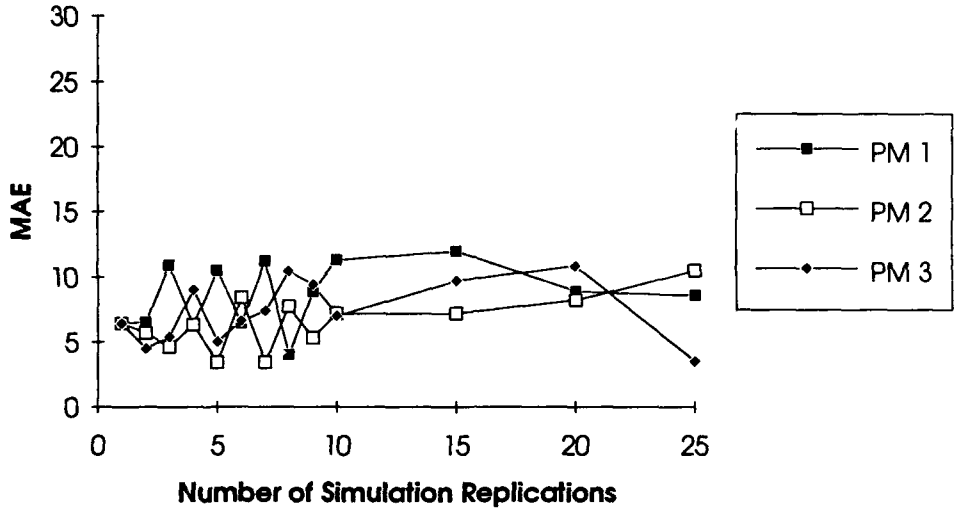


Figure 17 Training Set Results for Experiment 2 for Mean Cost

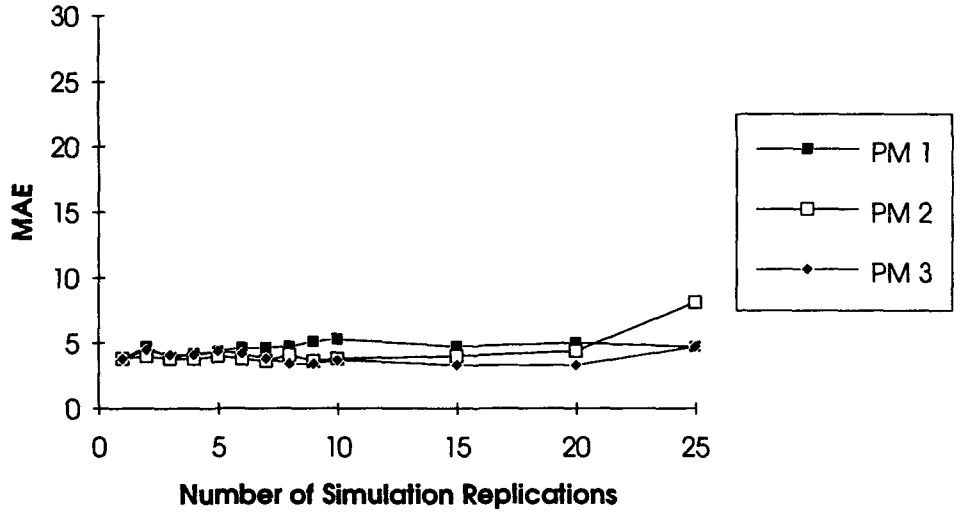


Figure 18 Training Set Results for Experiment 2 for Standard Deviation of Cost

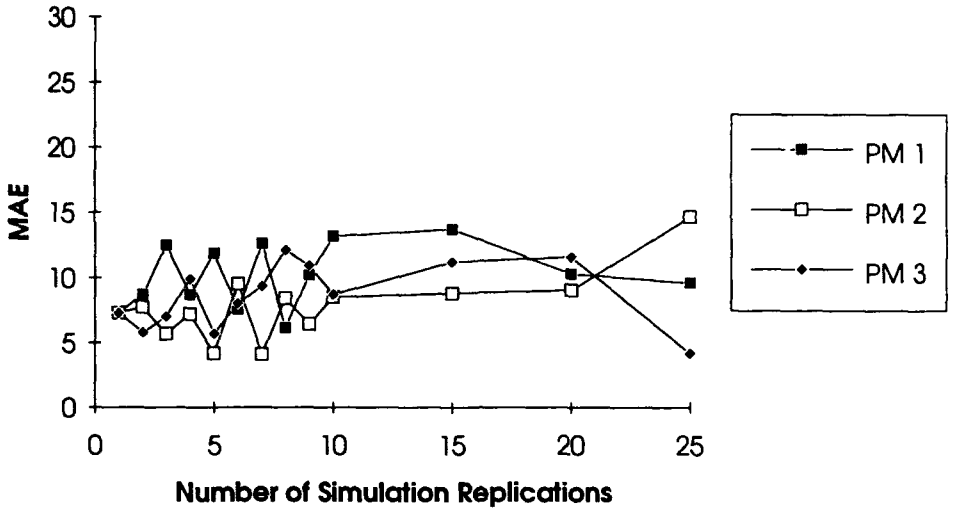


Figure 19 Training Set Results for Experiment 2 for Minimum Value of Cost

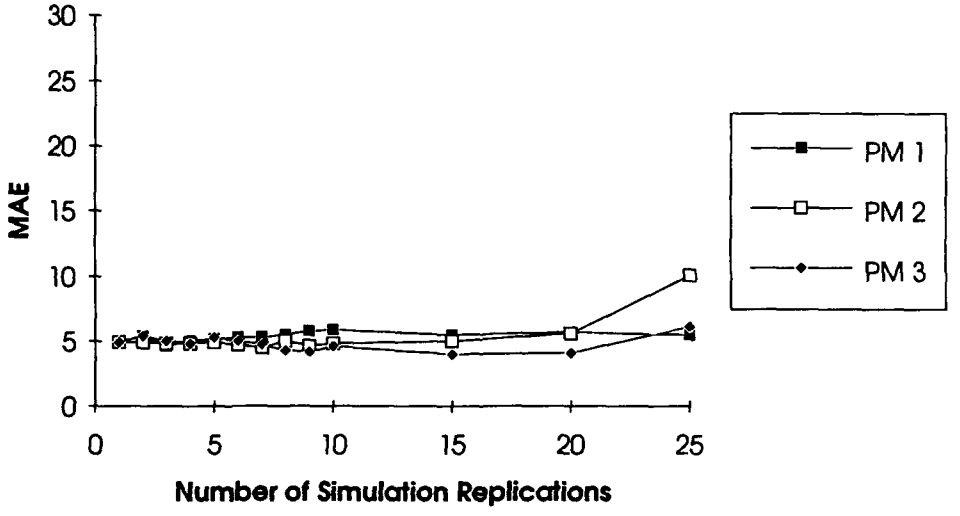


Figure 20 Training Set Results for Experiment 2 for Maximum Value of Cost

The amount of presentations (i.e., the number of training patterns shown to the network) required to terminate training for experiment 2 are given in Figure 21. It should be noted that the scale for Figure 21 differs considerably from the scale used on Figure 13 which is the corresponding figure from experiment 1. Many more presentations of the

data were needed to termi ining in experiment 2 than it did in experiment 1. In addition, many of the networks actually did not achieve the desired tolerance of 0.1 for all four of the output measures but instead terminated training by reaching the training termination criteria of 5,000 presentations of the data set to the ANN. Presentation methods 2 and 4 have more data than presentation methods 3 and 5, which have more data than presentation method 1. Consequently, they are correspondingly higher in terms of the number of presentations of data to the ANN during the training phase. Presentation method 1 was the only method that consistentl ged to the training tolerance of 0.1.

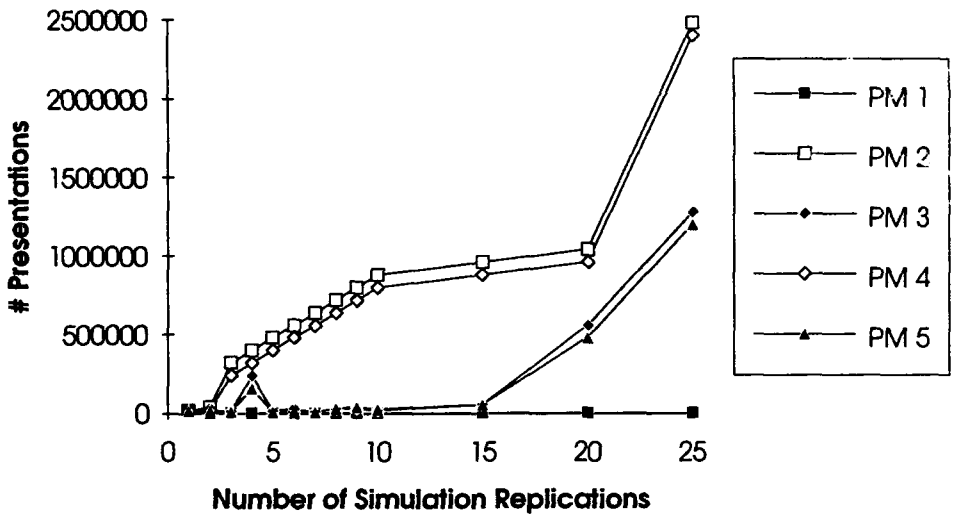


Figure 21 Presentations Required to Terminate Training for Experiment 2

The results for the test set of the three presentation methods for the mean, standard deviation, minimum, and maximum value of cost are given in Figures 22, 23, 24, and 25, respectively. The first observation that can be made from these figures is that in the vast majority of cases the largest error for all four of the measures of cost is found

with presentation method 1. There does not appear to be much of a difference in the performance of presentation methods 2 and 3. The second observation is that the erratic performance of the ANN in predicting mean and minimum cost that was present in the training data is also present in the testing data. Comparing the appropriate charts (i.e., Figure 17 versus 22, Figure 18 versus 23, Figure 19 versus 24 and Figure 20 versus 25), it is apparent that there is a larger degradation in the performance of networks on testing data compared to training data for mean value and minimum value of cost than for the standard deviation and maximum value of cost.

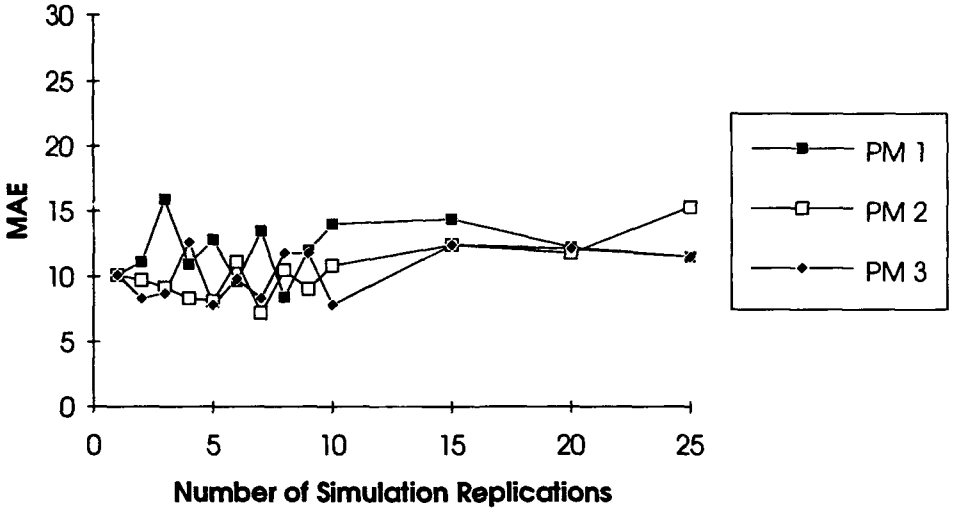


Figure 22 Test Set Results for Experiment 2 for Mean Cost

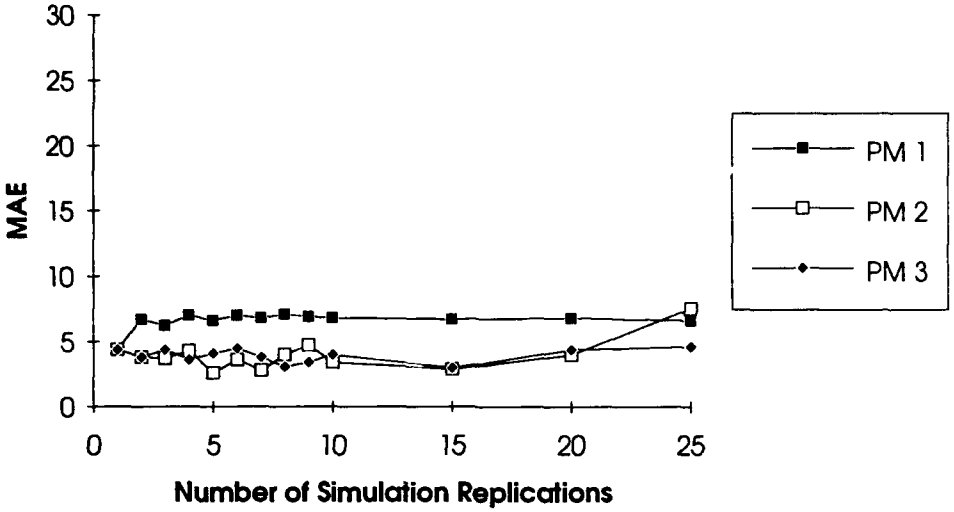


Figure 23 Test Set Results for Experiment 2 for Standard Deviation of Cost

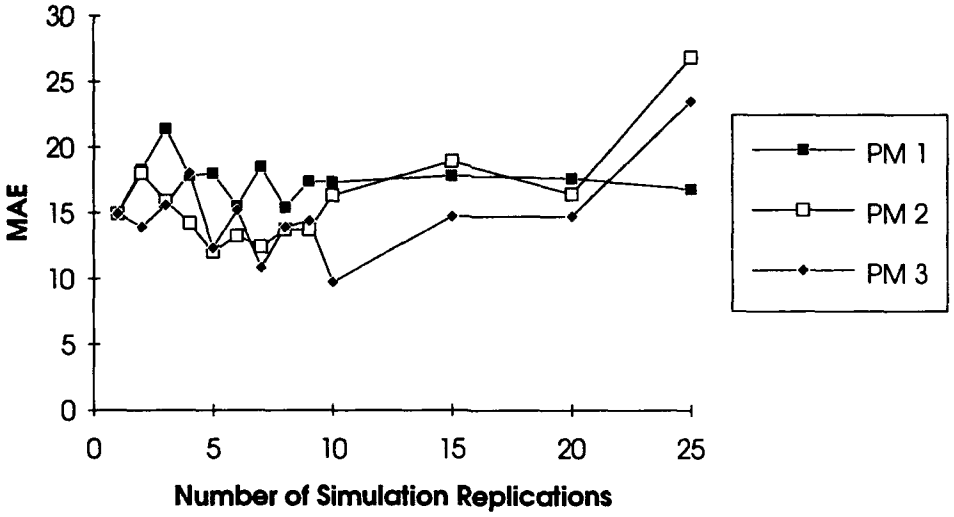


Figure 24 Test Set Results for Experiment 2 for Minimum Value of Cost

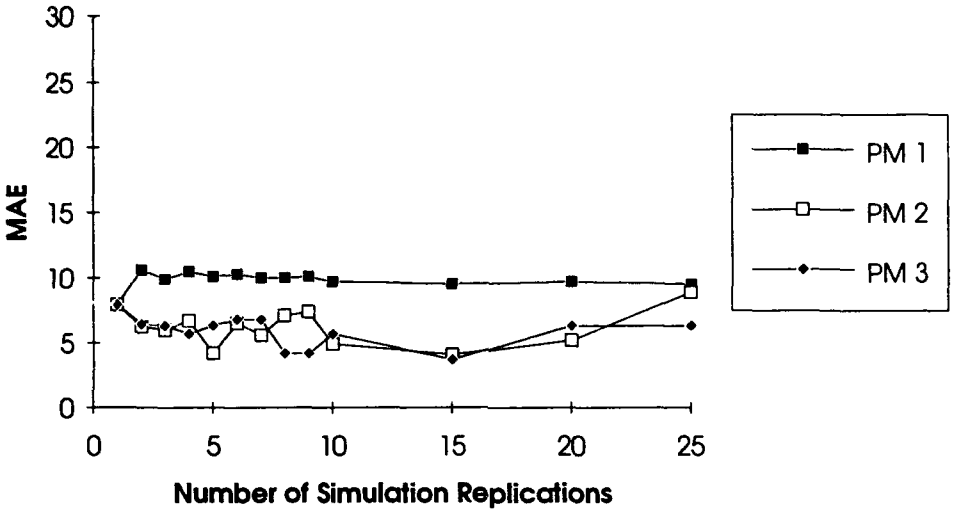


Figure 25 Test Set Results for Experiment 2 for Maximum Value of Cost

Experiment 1 and 2 both used ANN to predict mean cost of operating the inventory system for 120 months. The direct comparison of the results from these two experiments on predicting the mean value of cost for presentation methods 1, 2 and 3 is made in Figures 26 through 28 for the training set and in Figures 29 through 31 for the test set. The only truly valid comparison that can be made between the first two experiments is with presentation method 1, since it was the only presentation method that converged to the training tolerance in both experiments. It is apparent from Figures 26 through 28 that the approach used in experiment 1, having the ANN predict just one output, is much more stable for the training set than the approach used in experiment 2, which had the ANN predict four different outputs. It is also apparent from Figures 29 through 31 that the approach used in experiment 1 is much more stable for the test set than the approach used in experiment 2. Thus, it appears from these results that trying to predict single outputs only performs better than the multiple output approach when the number of simulation replications is large. The reason this has occurred is that, even though the training tolerance was the same for this measure of cost for both experiments 1

and 2, the networks for experiment 2 had to meet the training tolerance for an additional three measures. Since the single output ANNs all converged for all five presentation methods, it appears that there is room for additional training to take place by just reducing the training tolerance below 0.1. On the other hand, the multiple output ANN from experiment 2 did not consistently converge within the allowable 5,000 runs through the training data. Therefore, it appears that there would be little advantage to reducing the training tolerance below 0.1 when training on multiple outputs without lengthening the maximum number of epochs.

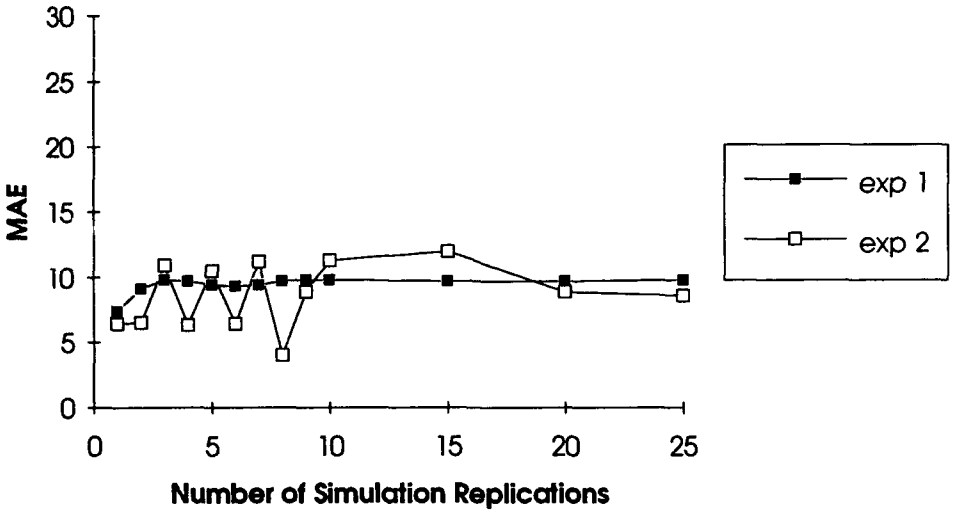


Figure 26 Comparison of Experiment 1 and Experiment 2 Training Set Results for Predicting Mean Value of Cost (C) for Presentation Method 1

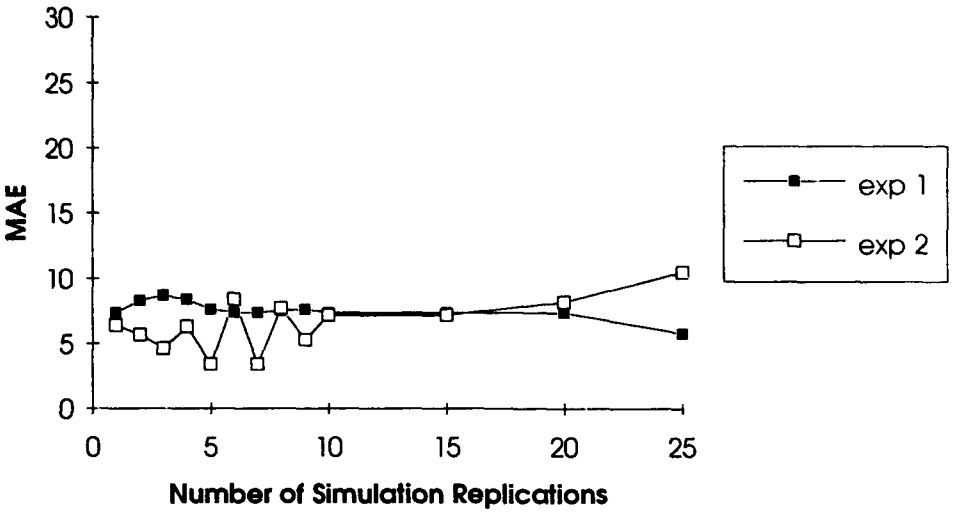


Figure 27 Comparison of Experiment 1 and Experiment 2 Training Set Results for Predicting Mean Value of Cost (C) for Presentation Method 2

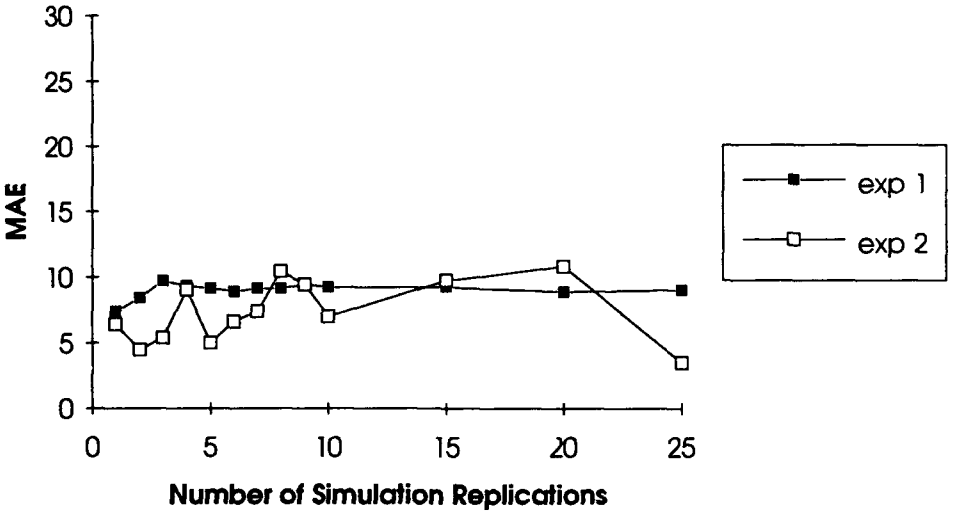


Figure 28 Comparison of Experiment 1 and Experiment 2 Training Set Results for Predicting Mean Value of Cost (C) for Presentation Method 3

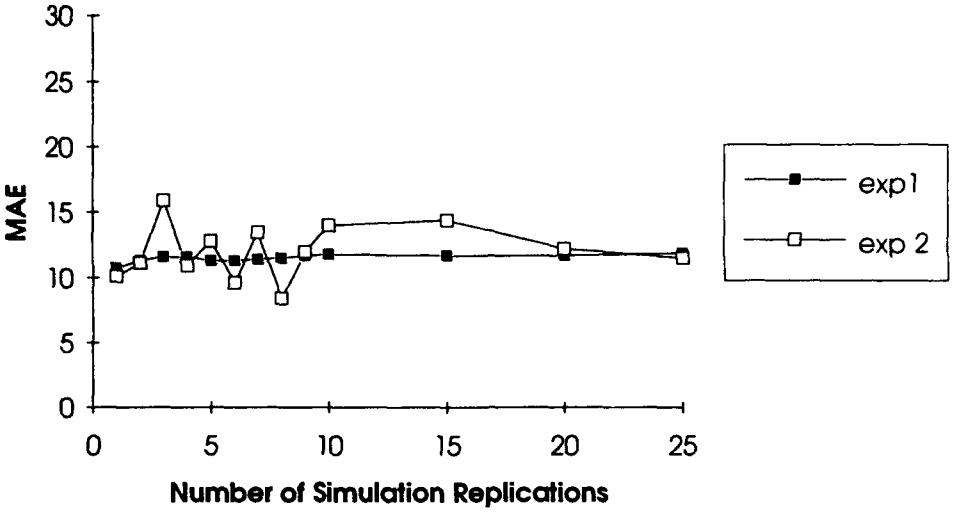


Figure 29 Comparison of Experiment 1 and Experiment 2 Test Set Results for Predicting Mean Value of Cost (C) for Presentation Method 1

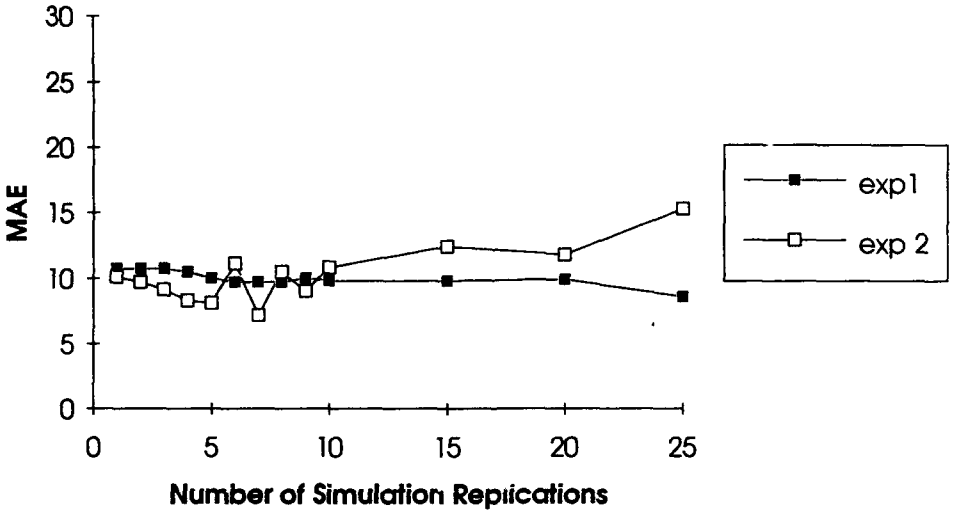


Figure 30 Comparison of Experiment 1 and Experiment 2 Test Set Results for Predicting Mean Value of Cost (C) for Presentation Method 2

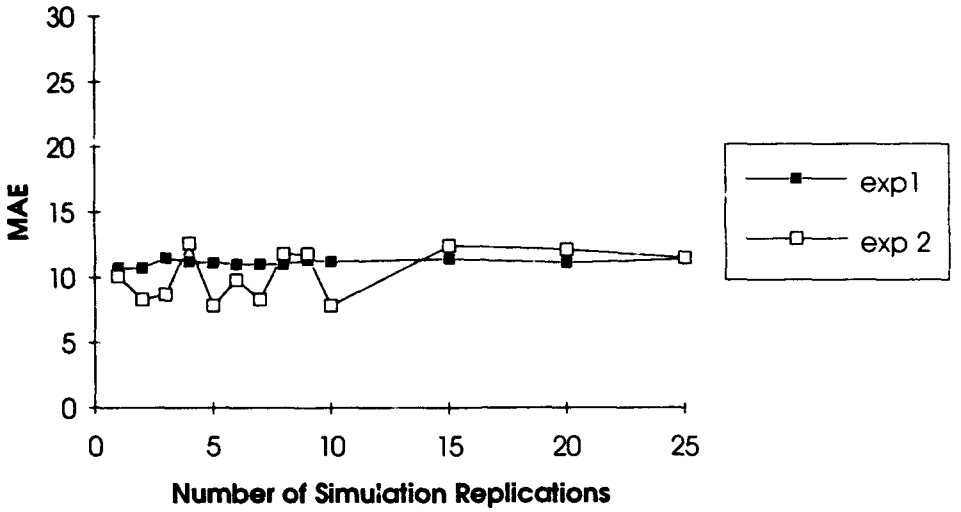


Figure 31 Comparison of Experiment 1 and Experiment 2 Test Set Results for Predicting Mean Value of Cost (C) for Presentation Method 3

Since stable predictors are preferable to unstable predictors, in general, the main conclusion to be derived from experiments 1 and 2 is that the approximation of multiple simulation output measures should be done with one ANN for each output measure, rather than one ANN for all of the output measures.

A second conclusion is that the method used in these two experiments for selecting the best network for each presentation method and set of training data is inadequate. In these experiments, it appeared that presentation methods 2 and 4, which used all of the simulation replications, produced better ANN. However, these presentation methods also did not consistently converge in experiment 2 and terminated training at an arbitrary predetermined number of runs (5,000 in this case) through the training data. This arbitrary stopping point is 5,000 steps away from a random starting point on the error surface that the ANN is trying to minimize and as a result may not be very close to the minimum error. While the lack of convergence in experiment 2 may have been due to trying to predict four

different output values, the following discussion shows that it could be due to another problem. That is, by virtue of the stochastic nature of computer simulations, there are different values produced by the computer simulation for the output of a specific combination of input parameter settings. For any given set of training data, there is at least one input parameter setting that has the largest difference between its multiple outputs, say MAXRANGE. If the desired training tolerance is smaller than MAXRANGE/2 then the network will fail to converge if all of the simulation output replications (i.e., presentation methods 2 or 4) are used as the training set. Thus, even though in these first two experiments presentation methods that use all of the replicated data did better than the presentation method that used the averages, it is quite possible that for a particular training tolerance level the presentation methods could not converge. The result would then be the final network, which in a sense is just a random point on the path from the starting point to the minimum on the error surface. There is no guarantee that such a point would be a very good point. In addition, if the training tolerance is small enough, it is possible for presentation method 1 to not converge within a pre-specified number of runs through the training data.

One way to avoid this problem is to pick a particular architecture for the ANN, use the termination criterion of "maximum number of runs" and write the results of the training performance to a file after each run through the training data. A search through the training results file will determine which run through the data produced the network with the best performance on the training set. Training without testing would then be conducted for the number of runs required to reach the best network. This procedure will be referred to as "best net training" and is used throughout the remainder of the dissertation. Another procedure that is similar is called "test and save" in which the

network is tested at pre-specified intervals and the networks are saved to individual files. If the networks are saved after each training run through the data, then the networks resulting from "best net training" and "test and save training" will be the same. Using the "test and save" training procedure does not require a second training session to obtain the weights of the best network. However, with the "test and save" procedure, it takes a lot of time to write the individual networks to different files, it takes a lot of memory to hold all of the files, and if the interval between testing networks is larger than one, then there is no guarantee of finding the best network. For these reasons "test and save" was not used in this research.

Further, adding just one example of the average value to the training set did not seem to help the learning process (i.e., presentation method 2 seemed to perform almost exactly like presentation method 4 and presentation method 3 seemed to perform almost exactly like presentation method 5). Therefore, presentation methods 2 and 3 were not considered in the remainder of the dissertation work. Also, presentation method 5 was bounded by presentation methods 1 and 4 in the sense that the networks created by presentation method 5 produced MAE that fell consistently between the MAE produced by networks developed using presentation methods 1 and 4. Therefore, presentation method 5 was not considered in the remainder of the dissertation.

One possibility of future research is to examine various increases in the number of copies of the mean value being added to the training set.

4.4 Synopsis of Conclusions from Initial Experiments on Inventory System

The following conclusions were derived from the experiments conducted in this chapter.

1. ANN should be used to perform interpolations rather than extrapolations from the training set.

2. Adding the additional data point of the average value of the output for each parameter setting provides little if any benefit in developing ANN. That is, there appears to be very little difference between presentation methods 2 and 4 or between presentation methods 3 and 5.

3. It is better to have several ANN, each predicting only one computer simulation output measure rather than having one ANN that is used to predict several measures.

4. There is insufficient evidence from these preliminary experiments to suggest that any one of the presentation methods is definitively better than the rest. The presentation method that tended to be the quickest (presentation method 1) and the presentation method that tended to produced the most accurate ANN (presentation method 4) will be considered in the remaining experiments.

5. The method used in experiments 1 and 2 for selecting the best ANN can be improved. Rather than limiting the possibilities to a "converged to the training tolerance" or a "reached training termination criteria" network, the results after each run through the training set should be saved. Searching through the resultant file would enable the "best

trained net" to be found. Retraining the initial network without testing and writing results to a file would permit the "best trained net" to be obtained. This is called the "best net training" approach to training ANN.

4.5 Summary

This chapter contains a discussion of the (s,S) inventory system which is used as a vehicle for developing an approach to building ANN metamodels of computer simulations. A three dimensional visual comparison between adirect simulation, a second-order regression metamodel, and an ANN metamodel demonstrated that for this problem the type of regression models used in response surface methods are not as accurate as ANN metamodels. The two experiments discussed in this chapter used two input parameters, s and d, and one output measure, cost. The first experiment examined various methods of presenting the simulation data to ANN. The result of the first experiment is that the networks trained on all of the individual replications of the computer simulation performed better than networks trained on just the average values or on half of the data closest to the averages. The second experiment examined the issue of predicting multiple outputs with one ANN or predicting with several ANN, each of which predicts a single output. By comparing the results of the ANN developed in the first and second experiments it is apparent that there is a confounding of learning is taking place when trying to predict multiple outputs with one ANN. The conclusion to be drawn is that it is better to develop separate networks when trying to predict multiple outputs. The final result of the experiments discussed in this chapter is the development of the "best net training" approach to developing ANN metamodels.

5.0 DEVELOPMENT PROBLEM - FINAL SET OF EXPERIMENTS IN APPROXIMATING AN (s,S) INVENTORY SYSTEM

The experiments in this chapter examine the ability of the ANN approximation method to handle increased model complexity in terms of the number of input parameters. To increase the complexity of the inventory model, the "controllable" input parameters k (setup cost) and u (underage cost) were added to the existing model with the other "controllable" input parameters of s (reorder point) and d (reorder quantity). This chapter focuses on estimating both the mean cost and variance of mean cost of inventory plans.

Most users of discrete event stochastic simulations are interested in estimating both the expected value and the variability of that expected value for specific combinations of values of input parameters. In stochastic simulation, the expected value (arithmetic mean) and the variance can be calculated as a by-product of multiple simulation runs. In a neural network metamodel of the type proposed in this research, outputs are deterministic, i.e., there is no attempt to replicate the stochastic aspects of the simulation. However, it is desirable to calculate a measure of the variability, as well as the expected value, for any particular response. Using the expected value and variance together allows for the construction of statistical prediction and confidence intervals for any system output. The capability to estimate both expected value and variance is provided by estimating each by a separate metamodel. Thus, for a given combination of input values, one neural network metamodel estimates the mean cost of the inventory plan, while another neural network metamodel estimates the variance of the mean cost.

5.1 Experiments with Four Simulation Input Parameters

The following experiments (3 through 6) were performed with the four input parameter inventory computer simulation. First, the number of hidden nodes needed to predict the simulation output is determined in experiment 3. In experiment 4 the mean cost of the (s,S) inventory system is predicted using ANN and is used to examine the tradeoffs between increasing the number of replications and increasing the number of data points. In experiment 5 the variance of the mean cost of the (s,S) inventory system is predicted using neural networks. In experiment 6 the ANN metamodels are used to make prediction intervals for the cost of the (s,S) inventory system.

For this experiment, and all subsequent experiments, the only presentation methods used were presentation method 1 (average of output data) and presentation method 4 (all individual replications). In this problem mean cost is calculated, for each particular input parameter setting, according to equation 5-1 and the variance of the mean cost, also called the squared standard error, is calculated according to equation 5-2, for ten replications.

$$\text{Mean} = \bar{C} = \frac{\sum_{i=1}^{10} C_i}{10} \tag{5-1}$$

$$\text{Var}(\bar{C}) = (SE)^2 = \frac{\sum_{i=1}^{10} (C_i - \bar{C})^2}{\frac{9}{10}} \tag{5-2}$$

The data used to train and test the ANN for the experiments on the 4 input parameter inventory system simulation was obtained using the SIMAN computer

simulation programs given in Appendix B, Figures B1 and B2. This simulation is identical to the one used for the 2 input parameter inventory system except that the code was modified to accommodate the larger number of input parameters. In these experiments a reparameterization of the factor u was used to prevent having unreasonable combinations of u and k. The reparameterization was to let w = k/u. In the 2 input parameter inventory computer simulation the parameter k was always at the value $32 and the input parameter u was always equal to the value $5 (and so the parameter w was 32/5, or 6.4).

The values of the four input parameters selected for training and testing neural networks are shown in Table 9. Using ten values of s, ten values of d, five values of k and five values of w, a total of 2,500 different combinations of input parameter values were simulated ten times to obtain a total of 25,000 replications of training data. To examine the tradeoffs of more data points versus additional replications, the training data was divided into smaller non-disjoint sets. Table 9 shows several sets of values for each parameter. The parameter s, has three sets of values, one set of size 2, one set of size 4 and one set of size 10. Similarly, d, k and w have three, four, and four sets of values respectively. Thus, there are 144 (3x3x4x4) combinations of the different sets of values of the input parameters. Table 10 shows the thirteen combinations of the sets of training input parameter values that were considered in the experiments involving the 4 parameter inventory system computer simulation. Each training set is a subset of any training set that is below or to the right of it in Table 10. The one exception to this rule is training set J, since it is a combination of training sets E and I, each of which contains the training set A, with one of the two sets of training set A removed. Training set J was included to examine the advantage of having detailed information about each input parameter without the disadvantage of having very large amounts of data, as is the case with training set M.

Table 9 Training and Testing Values for 4 Input Parameter Inventory Simulation

Input Parameter/ Data Type	Number of Values	Parameter Values
s		
train	2	20 80
train	4	20 40 60 80
train	10	20 27 33 40 47 53 60 67 73 80
test	5	10 30 50 70 90
d		
train	2	20 80
train	4	20 40 60 80
train	10	20 27 33 40 47 53 60 67 73 80
test	5	10 30 50 70 90
k		
train	2	16 80
train	3	16 48 80
train	4	16 32 64 80
train	5	16 32 48 64 80
test	6	8 24 40 56 72 88
w		
train	2	4 17
train	3	4 10.5 17
train	4	4 8 13 17
train	5	4 8 10.5 13 17
test	6	3 6 9 12 15 18

s = reorder point d = reorder quantity
k = setup cost w = parameterization of u-underage cost, where w = k/u

Table 10 Training Sets for 4 Input Parameter Inventory Simulation

Number of Values of Input Parameters	2 values of s 2 values of d	4 values of s 4 values of d	10 values of s 10 values of d
2 values of k 2 values of w	A (16)	D (64)	I (400)
3 values of k 3 values of w	B (36)	F (144)	K (900)
4 values of k 4 values of w	C (64)	G (256)	L (1600)
5 values of k 5 values of w	E (100)	H (400)	M (2500)
J (484) = E+I-A			

(Numbers in parentheses in the table indicate the number of points in the training set)

Due to computer memory restrictions, the computer simulation program was run in separate batches of 10 replications for the training data and 20 replications for the testing data. To obtain independent replications, the random number streams shown in Table B1 were used for the different batches. To reproduce the computer simulation results from SIMAN that were obtained in this research would require putting the input data in an ASCII file in the same order that is shown in Table B2 in Appendix B. In Table B2, all of the parameters begin with the smallest values. The first three parameters are then held fixed and the values for parameter w are increased from the smallest to the largest value. Then k is increased to its next highest value and the process is repeated to the parameter w. This iterative process is repeated for all values of k, and then all values of d and then all values of s. The process is repeated until all possible combinations are achieved. The results of the first 90 data points for the 10 replications of the training set are shown in Table B2. All of the data for the training sets was obtained by running the simulation on training set M, and then dividing the results appropriately to form the other training sets. An example of one of the training sets, specifically training set A, is shown in Table 11 with the results of 10 replications of the computer simulation in terms of the mean cost and the variance of the mean cost. Training set A is a 2^4 design which is the standard full factorial design used in traditional response surface methods. Other more sophisticated designs such as Box Behnkin and star point designs may be more appropriate if optimization of the response surface is the goal. Training set F is shown in Table B3 in Appendix B. Training set F is a $3^2 \times 4^2$ design. The data has been shuffled in both Table 11 and Table B2 for ANN training purposes. M, the largest training set is a $10^2 \times 5^2$ design.

Table 11 Example of 4 Parameter Inventory Training Set - (Training Set A)

Training Data Point	Input Parameters				Output Values of Cost	
	s	d	k	w	$\overline{C}$	Var($\overline{C}$)
1	20	80	80	17	140.277	0.953
2	80	80	80	17	192.377	0.664
3	20	80	80	4	161.124	6.490
4	80	80	80	4	192.633	0.618
5	20	80	16	17	118.079	0.210
6	80	80	16	17	175.904	0.737
7	20	80	16	4	121.533	0.772
8	80	80	16	4	176.024	0.397
9	20	20	80	17	161.961	2.011
10	80	20	80	17	200.964	2.681
11	20	20	80	4	217.053	11.277
12	80	20	80	4	202.047	2.943
13	20	20	16	17	98.33	0.921
14	80	20	16	17	152.539	0.579
15	20	20	16	4	109.109	0.534
16	80	20	16	4	153.05	0.425

The test sets for these experiments were constructed using the combinations of the test set parameter values for each of the input parameters given in Table 9. There are 900 (5x5x6x6) points in the entire test set. Each point in the test set can be categorized in terms of the number of parameters whose values are beyond the range of any of the parameter values in the training sets. The result is a division of the test set into the five groups of data listed in Table 12. An example of the input parameters for a test set and the simulation results of mean cost and variance of the mean cost, are given in Table 13 for the test set with all four values of the input parameters external to the training set. Test set 0, from Table 12 is a wholly interpolative test set. The results of the simulation runs for the test set with 0 parameters external to the training sets are shown in Table B4 in Appendix B.

Table 12 Subdivisions of Test Set for 4 Parameter Inventory Simulation

Test Set (Number of parameters with value external to training set values)	Number of Points in Test Set
0	144
1	336
2	292
3	112
4	16
TOTAL	900

Table 13 Test Set with 4 External Values for 4 Parameter Inventory Simulation

Testing	Input Parameters				Output Values of Cost	
Data Point	s	d	k	w	$\overline{C}$	Var($\overline{C}$)
1	10	10	8	3	115.13	2.06
2	10	10	8	18	87.92	0.71
3	10	10	88	3	518.13	100.11
4	10	10	88	18	219.77	6.19
5	10	90	8	3	118.09	0.62
6	10	90	8	18	111.30	0.51
7	10	90	88	3	216.72	19.20
8	10	90	88	18	143.18	1.57
9	90	10	8	3	151.95	0.33
10	90	10	8	18	151.84	0.25
11	90	10	88	3	230.04	0.50
12	90	10	88	18	230.01	0.62
13	90	90	8	3	188.05	0.49
14	90	90	8	18	188.03	0.49
15	90	90	88	3	207.83	0.63
16	90	90	88	18	207.92	0.72

A traditional backpropagation training algorithm was used with a smoothing factor and a unipolar sigmoidal transfer function as given in equation 3-1, with a training tolerance of 0.02. For some prediction problems it is difficult for the ANN to achieve very high values or very low values of the target output due to the undershoot phenomenon.

The default setting for the range of normalization of both the inputs and outputs in the BrainMaker package is to use the minimum and maximum values observed in the training data. In these experiments, the test data extends beyond the range of the training data both in terms of inputs and outputs. Thus, for this research the range of normalization for the input values was extended so that the minimum value was set at 10% of the range lower than the minimum value of the train and test sets combined and the maximum value was set at 10% of the range higher than the maximum value of the train and test sets combined. For instance, for the input parameter s, the training set values had a minimum of 20 and a maximum of 80, while the test set had a minimum of 10 and a maximum of 90. Since the range of the combined train and test sets was 80 (90-10), BrainMaker used a minimum value of 2 (10 - .1 x 80) and a maximum value of 98 (90 + .1 x 80) to scale the input parameter s. The factor of 10% of the range beyond the minimum and maximum values found in the test set was used after several trials using factors of 0%, 10%, and 20%. Similar trials were conducted to examine the factor to use for the output values with the result that a 10% factor for adjusting the minimum and maximum of the mean cost of operating the inventory system performed best. For predicting the variance of the mean the factor used to adjust the range of the inputs remained at ±10%, but the target output used 10% lower than the minimum and 20% higher than the maximum since these values yielded the best results. The remainder of these experiments used these adjustments to the scaling factors for both the inputs and outputs of the ANN.

5.2 Experiment 3: Determining the Number of Hidden Nodes Needed to Predict the Simulation Output Measure

In this experiment the ANN architecture has four input nodes, two hidden layers with a varying number of nodes, and a single output node. The objective of this

experiment was to determine how many nodes to use in the hidden layers. In this experiment training sets A and M from Table 10 were used. These training sets were the smallest and largest training sets, with 16 and 2500 data points respectively. A total of six ANN were developed using these two training sets. Two of the ANN were developed using the mean and the individual replications of training set A. Four of the ANN were developed using the mean and the individual replications of training set M with two of these ANN using shuffled data and two of them using unshuffled data.

Each of the networks in this experiment were trained for 50 epochs. The networks were evaluated after each epoch, and the one which performed best on the training set was saved as the final trained network. The average number of epochs required to reach the minimum training error was 26.

The results on the test set in terms of Mean Absolute Error for the ANN trained on the unshuffled data of set M are shown in Figure 32. As can be seen in the figure, the best number of hidden nodes is five for both the averages and individual replications. After this initial experiment, it was clear that the number of hidden nodes that would work best for this data was between 2 and 10, and so, the succeeding examinations of the number of hidden nodes was restricted to this range. After examining Figure 32, it became apparent from the erratic behavior of networks trained on individual replications that the ANN might have better and more stable performance if the training data was shuffled for such a large training set. The results for data set A and the shuffled and unshuffled data set M are provided in Figures 33 and 34. Figure 33 shows that all three of the ANN trained on averages achieved the smallest MAE with five hidden nodes. Figure 34 shows that two out of three achieved the smallest MAE with five hidden nodes and the

other achieved the smallest MAE with four hidden nodes for the ANN trained on individual replications. In addition, Figures 33 and 34 show that shuffling the data improves the results by reducing the test set MAE and for the individual replications, providing more stable performance. In all six cases good performance in terms of MAE was achieved using five hidden nodes.

Based on these results the following ANN architecture is used in the remaining experiments of predicting cost with the four input parameter inventory simulation: four input nodes, two hidden layers of five nodes each, and a single output node. In addition, since it was observed that the networks trained on data set A achieved their best level of performance at 50 epochs, which was the maximum number of epochs for this experiment, succeeding experiments increased the maximum number of epochs to 750.

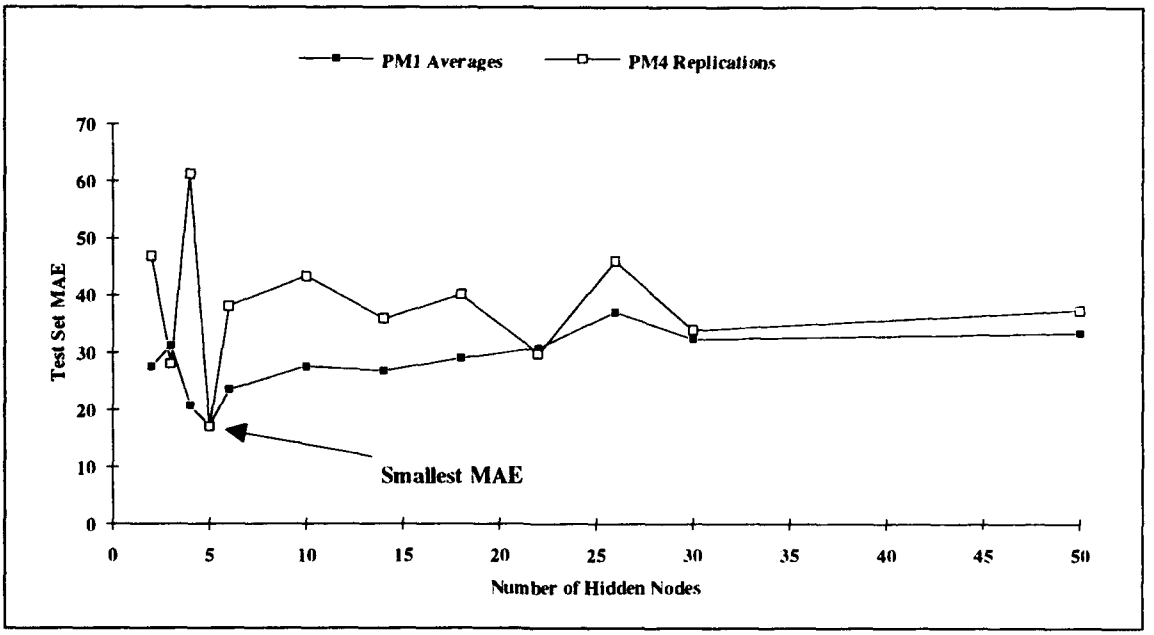


Figure 32 Results of Experiment 3 for Training Set M (Unshuffled Data)

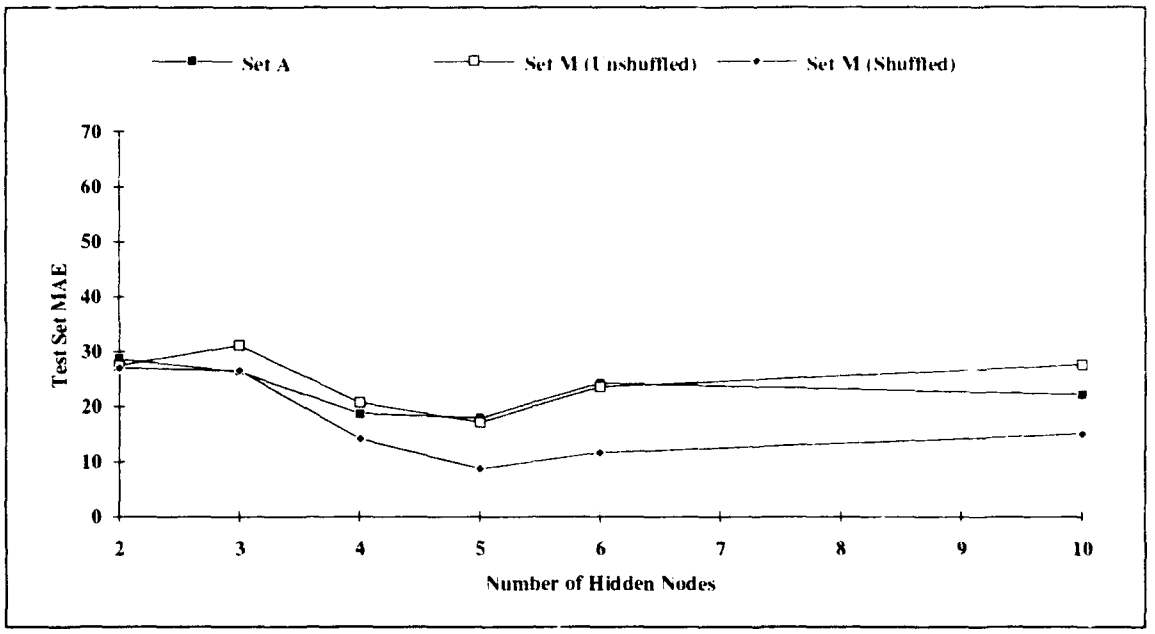


Figure 33 Results of Experiment 3 for ANN Trained on Averages (PM 1)

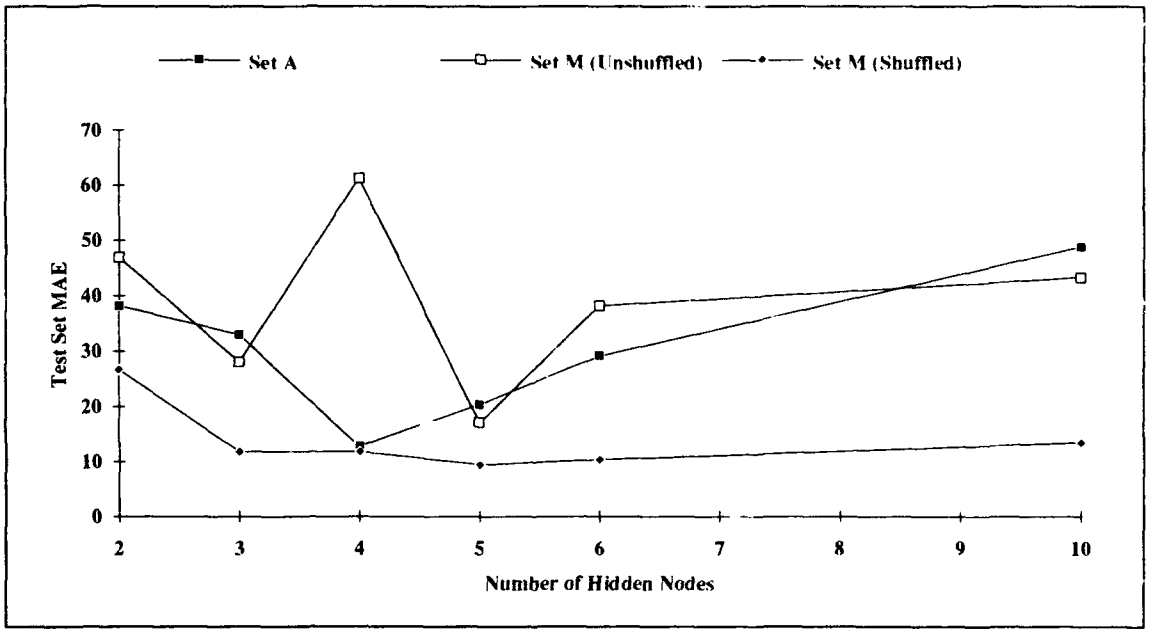


Figure 34 Results of Experiment 3 for ANN Trained on Individual Replications (PM 4)

5.3 Experiment 4: Predicting Mean Cost of the (s,S) Inventory Simulation

In this experiment the training data was presented to the network using presentation method 1 and presentation method 4. All 13 of the training sets shown in Table 10 were used to develop ANN to predict the cost of operating the inventory system. Each set of training data was also organized into three different subsets: the first two replications comprised the first subset, the first six replications made up the second subset, and finally, all ten replications were used in the third subset. Thus, a total of 78 (2x13x3) ANN were constructed for this experiment.

Each of the networks in this experiment were trained for 750 epochs. The networks were evaluated after each epoch, and the one which performed best on the training set was saved as the final trained network. The average number of epochs required to reach the minimum training error was 418 epochs for the networks trained on averages and 253 epochs for the networks trained on individual replications. Due to the larger individual replication data sets, this translated to an average number of presentations of each input data point to reach the best trained network of 418 for the networks trained on averages and 1,743 for the networks trained on individual replications. Several networks were trained to 7,500 epochs and in each case the best network was achieved within the first 750 epochs.

5.3.1 Examining Four Input Dimension ANN Results on a 2 Dimensional Surface

Before examining the results of this experiment, the following discussion compares how well the ANN trained using four dimensional input predicts the two dimensional surface of the ten replications of 420 points of direct simulation shown in Figure 9a. It should be noted that all 420 points plotted in Figure 9a had the same values for the

parameters k and w. The parameter k was set to 32 and the parameter w was set to 6.4. The closest values in training set F to these settings are with k equal to 16 or 48 and w equal to 8. Also there are only 16 different values in the (s,d) space in data set F. Table 14 compares the regression and ANN metamodels developed with the 36 points from Chapter 4, shown in Figures 9b and 9c respectively, with the ANN metamodel developed on the individual replications of training set F. Based on the three criteria of mean absolute error, maximum absolute error and variance of error, the ANN developed on training set F outperformed the regression developed with 36 points but did not do as well as the ANN developed with 36 points. Figure 35 shows the predictions made by the neural network developed for this experiment using the ten individual replications of data set F. In spite of the sparseness of the training data and its dissimilarity with the test set, the plot of predicted values for the ANN trained on the individual replications of training set F appears to be reasonably close to the direct simulation plots of 420 points shown in Figure 9a and appears to be at least as good as the plot constructed using the regression on 36 points shown in Figure 9b.

Table 14 Comparison of Chapter 4 and Chapter 5 Networks

Metamodel Method	**Regression**	**ANN**	**ANN**
Training Set	**Chapter 4 Set B**	**Chapter 4 Set B**	**Chapter 5 Set F**
Total Number of Training points	36	36	144
Number of Different (s,d) Training Points	36	36	16
MAE (Entire Test Set)	8.64	3.20	5.09
Maximum Error (Entire Test Set)	52.15	12.02	52.02
Variance of Error (Entire Test Set)	33.71	4.64	32.66
MAE (Internal Points)	9.00	3.12	3.21
Maximum Error (Internal Points)	23.33	8.29	9.57
Variance of Error (Internal Points)	24.91	4.09	4.57

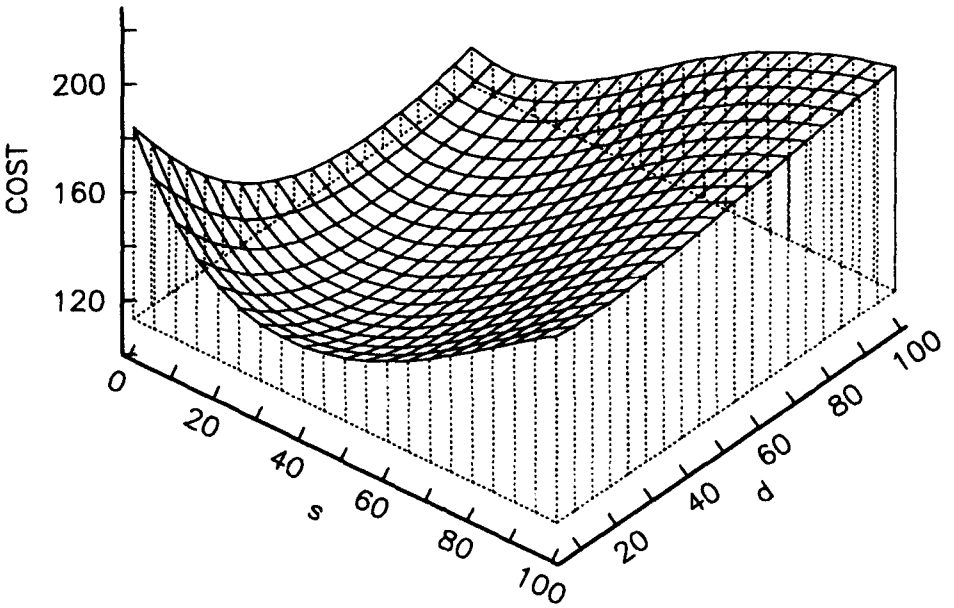


Figure 35 Surface Plot of Mean Cost Based on Training Set F

5.3.2 Results of Experiment 4

The training sets of average values had the advantage of being smaller and typically converged more quickly in terms of the total number of data presentations to the network than the training sets of individual replications. The plot in Figure 36 shows that all but one of the individual replications training sets took longer to reach the best trained network than for those nets trained on the average of the ten replications. Similar results were found for the nets trained on two and six replications.

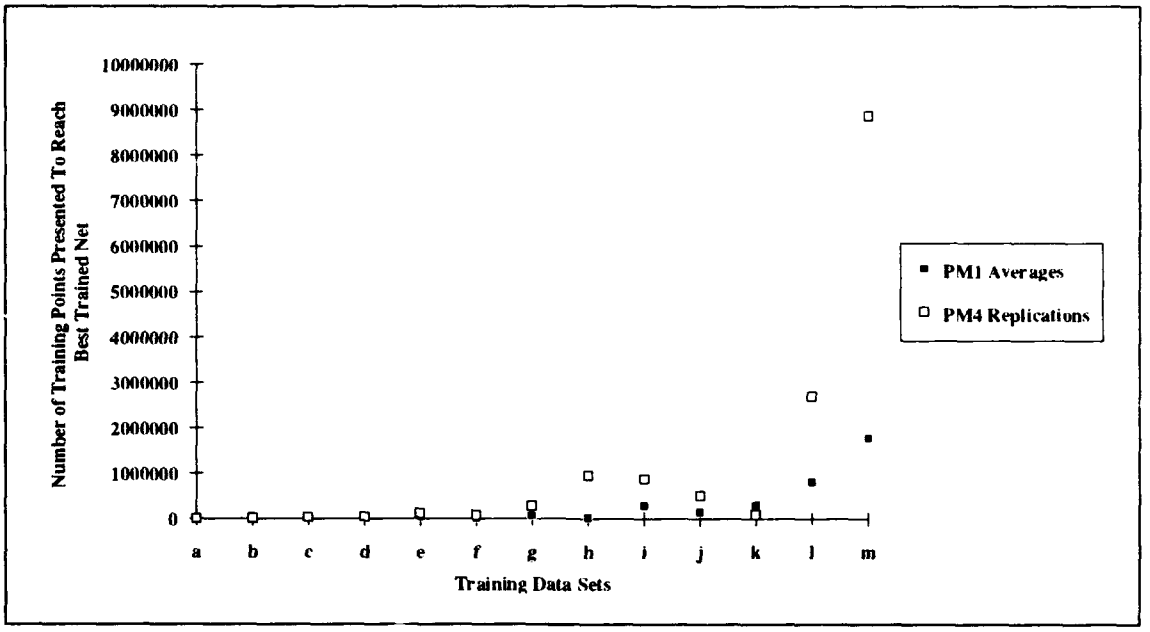


Figure 36 Number of Presentations of the Training Data To Reach the Best Trained Network in Experiment 4 for Training Sets Based on 10 Replications

One might expect to get the same results for predicting the mean cost of the inventory policies of the test set data from both types of presentation methods, except that the replication training would take much longer. This, in fact, did not happen. There were fundamental differences in the performance of the networks, depending on the method used to present the information to the networks during training. The individual replications networks were more consistent in their ability to accurately predict total cost for the test set. Initially this seemed counterintuitive. For the individual replications case, training could not expect to reach a pre-specified training tolerance for all points since for each training point there are ten (for the ten replication case) identical input vectors, each with a different target output. Thus, if the training tolerance is larger than half the distance between the minimum and maximum output values for a particular set of input parameter values, it will be impossible to correctly learn all ten of the outputs for that particular input parameter setting.

The output of the computer simulation for cost of the inventory system ranged in value from 88 to 518. The average cost of all the points in the test set was 159. Figures 37, 38 and 39 show the networks trained on individual replications typically doing much better than the networks trained on averages. All of the figures show the results in alphabetical order of the training sets which are also in non-decreasing order of the size of the training set. Figure 37 shows the results for the entire test set, while Figure 38 shows the results for the test set consisting of all points with either zero or one value external to the training sets and Figure 39 shows the results for all test points with either two, three or four values external to the training sets.

As can be seen in Figure 37 only two of the networks, training sets E and K, perform better with averages than with individual replications. Also as the number of data points is increased the MAE decreases except for training sets E and I. It is likely that training sets E and I do poorer than networks trained on fewer data points because they have too much information on some inputs. This can be seen by examining the data sets in Table 10. Training set E might have too much information about the parameters k and w. and not enough information about parameters s and d, while training set I might have too much information about the parameters s and d and too little information about parameters k and w.

The results in Figure 38 indicate that for a more interpolative test set, all training sets with at least as many points as training set F (144 points) do better than those trained on fewer than 144 points. For this test set, networks trained on averages only do better than networks trained on individual replications for data sets E and K.

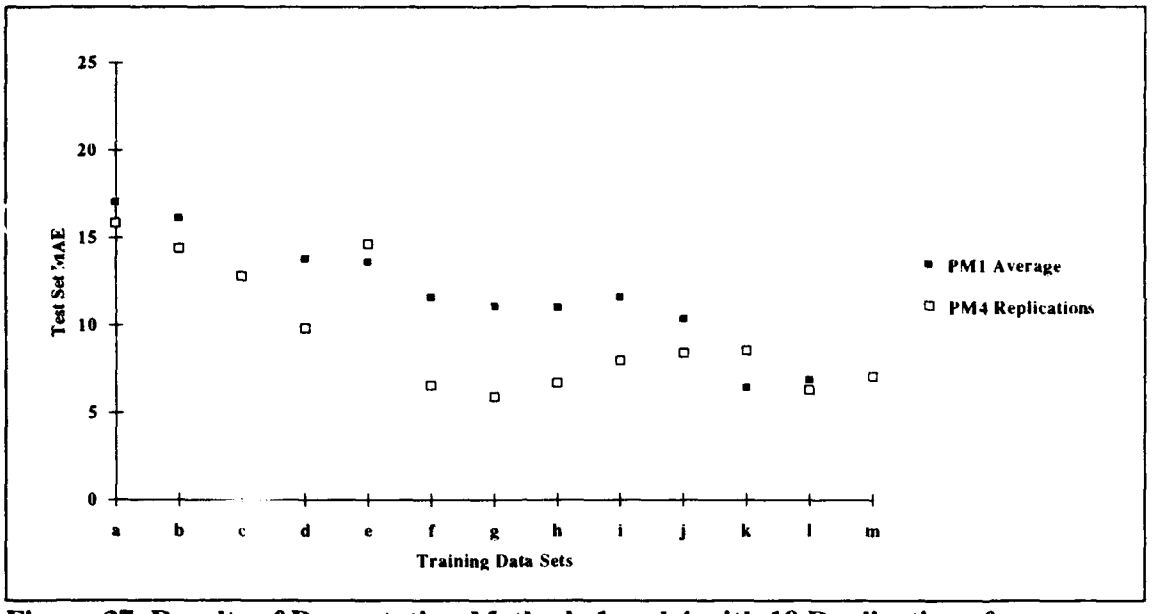


Figure 37 Results of Presentation Methods 1 and 4 with 10 Replications for Experiment 4 for the Entire Test Set

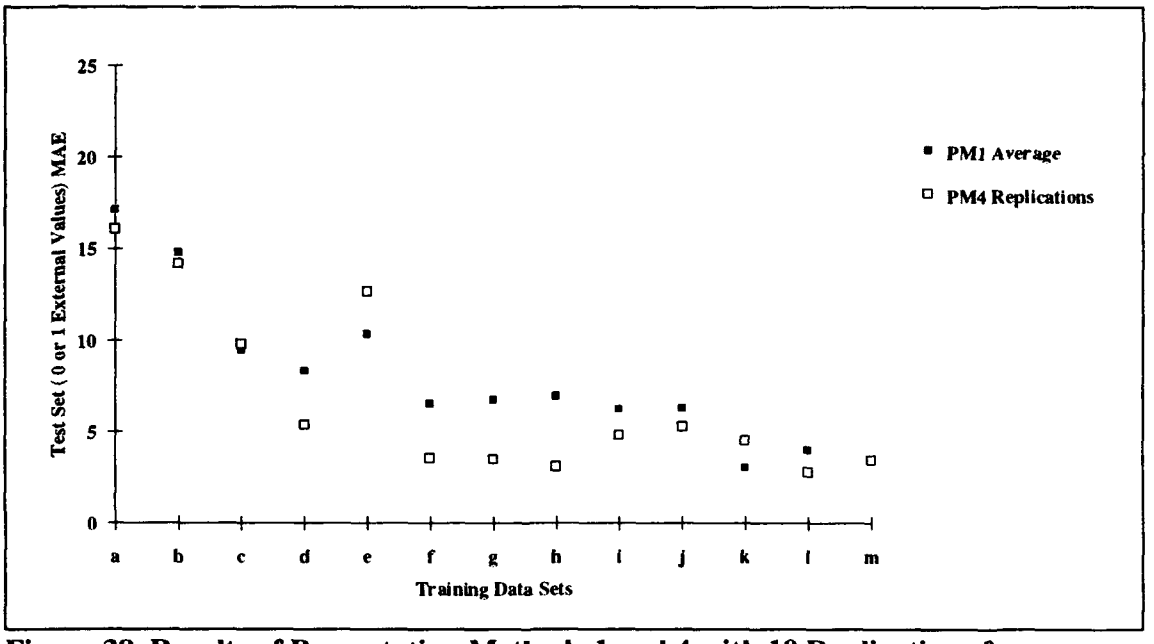


Figure 38 Results of Presentation Methods 1 and 4 with 10 Replications for Experiment 4 for Test Set with 0 or 1 External Values

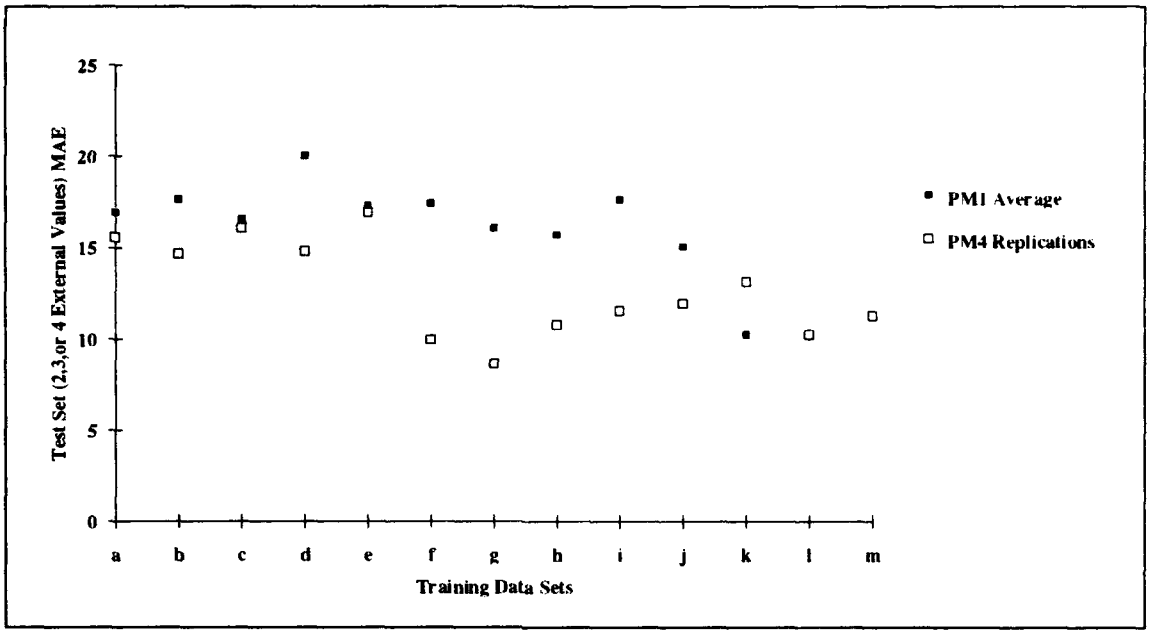


Figure 39 Results of Presentation Methods 1 and 4 with 10 Replications for Experiment 4 for Test Set with Two, Three, or Four External Values

It is expected that the less extrapolation is performed the better the ANN metamodels performance will be. With the exception of training sets A and B, all of the ANN metamodels do much better at predicting the mostly internal points of test sets with 0 or 1 external factors in Figure 38 than they do at predicting the test sets with two, three or four factors external in Figure 39. It should also be noted that the reduction in test set error resulting from additional data points is much greater for the interpolative test set than for the extrapolative test set. The reduction from training set A to training set M is approximately 75% (from 16 MAE to 4 MAE) in Figure 38 and is approximately 25% (from 16 MAE to 12 MAE) in Figure 39.

The results for the more extrapolative test set indicates that it takes considerable more training data to obtain a definitive reduction in the test set error than it did for the interpolative test set. Figure 39 shows that improvement occurs when the training set is at least as large as training set K (900 points). For this extrapolative test set, networks

trained on averages only do better than networks trained on individual replications for data set K.

For all of the test sets it appears from Figures 38 and 39 that networks trained on very little data (Training Sets A, B and C) or on a lot of data (Training Sets L or M) are not much different for the two data presentation methods. However, for the training sets from D through K there does appear to be a difference between training on averages and training on individual replications.

The result of increasing the number of replications at each point is shown in Figures 40 through 43. Figures 40 and 41 show the results for presentation method 1 (averages) with the entire test set and the test set with 0 factors external, respectively. Similarly, Figures 42 and 43 show the results for presentation method 4 (individual replications). All four of the figures demonstrate that training neural networks is a stochastic versus a deterministic process. Figures 40 and 41 show that there is not much benefit to increasing the number of replications when training on the averages. Figures 42 and 43 indicate that there is a slight benefit to increasing the number of replications when training the ANN is based on individual replications. For other problems the effect of additional replications could be much more pronounced. These results indicate that for this problem there is much more variability between the input data points than there is within the replications performed at a particular data point. It should be noted that the error on the purely interpolative test set as shown in Figures 41 and 43 is quite small for both presentation methods once sufficient data points (at least 144 points with data set F) are provided as the training set.

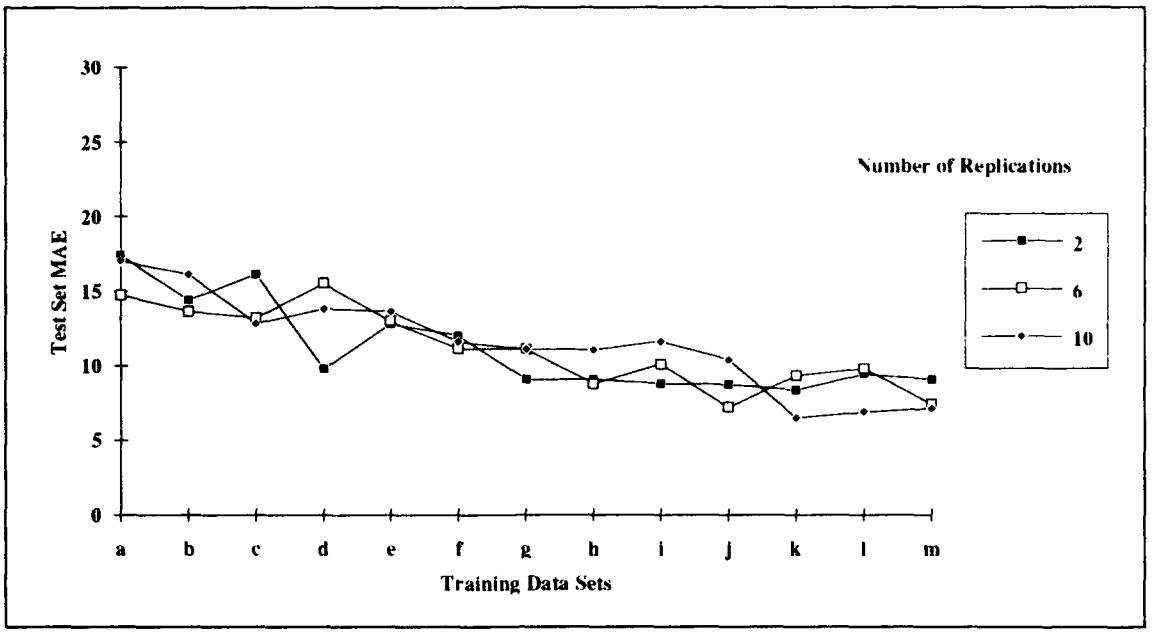


Figure 40 Results for Entire Test Set with PM 1-Averages for Varying Number of Replications in Experiment 4

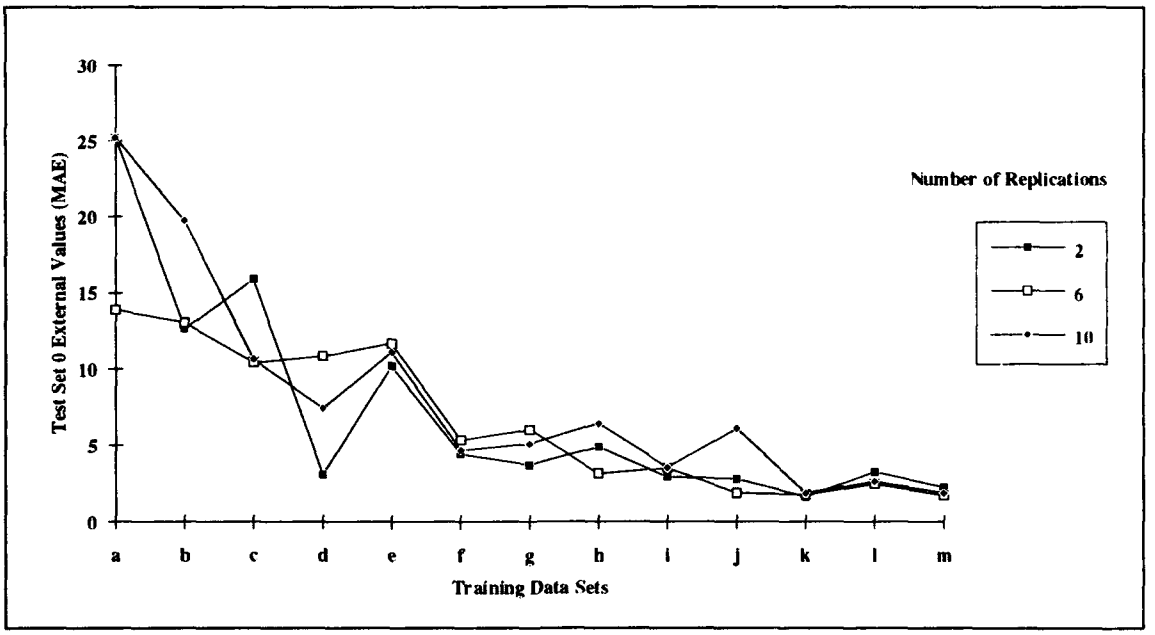


Figure 41 Results for 0 External Factors Test Set with PM 1-Averages for Varying Number of Replications in Experiment 4

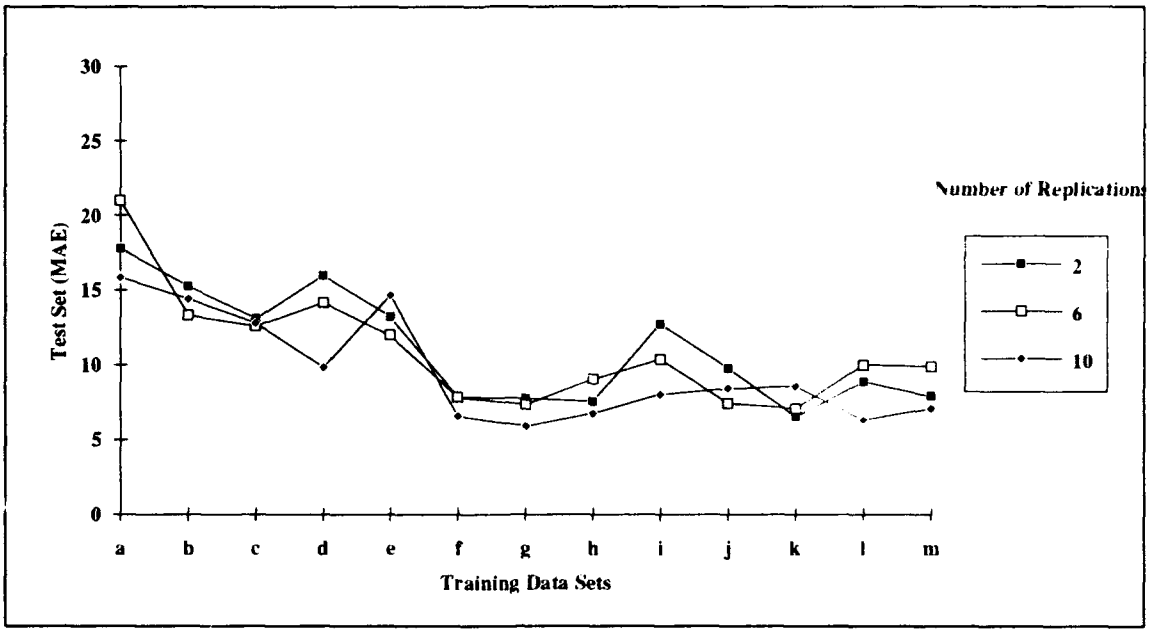


Figure 42 Results for Entire Test Set with PM 4-Individual Replications for Varying Number of Replications in Experiment 4

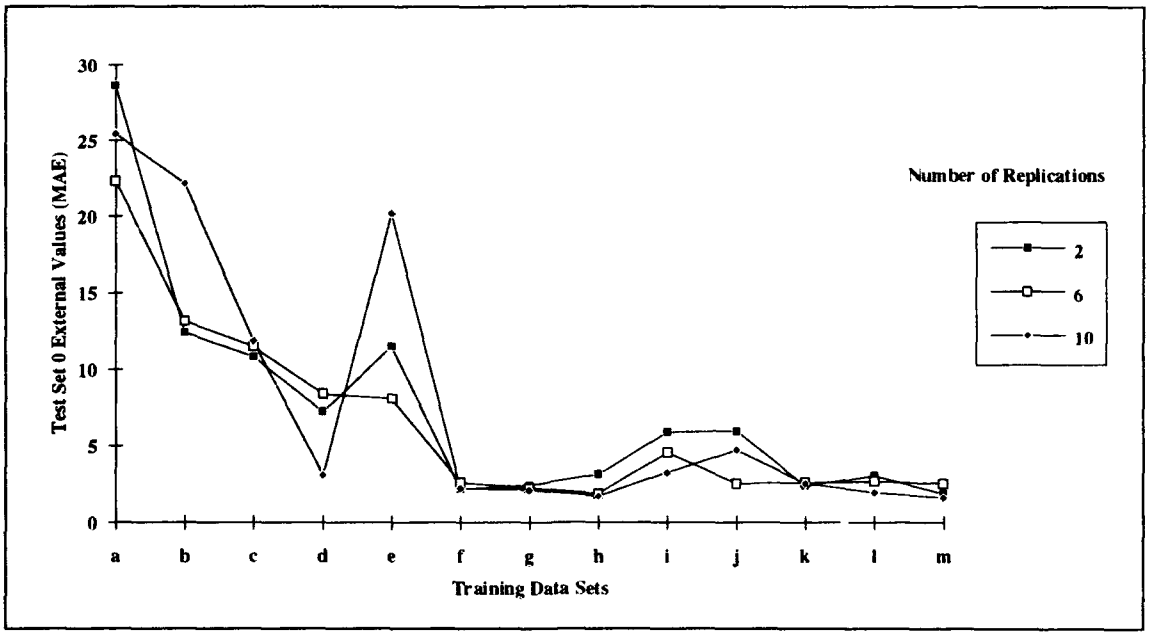


Figure 43 Results for 0 External Factors Test Set with PM 4-Individual Replications for Varying Number of Replications in Experiment 4

5.4 Experiment 5: Predicting the Variance of Mean Cost of the Four Parameter Inventory Simulation

This experiment is designed to predict the variance of the mean cost of operating the inventory system as predicted by the computer simulation. Note that variance as well as the mean of the computer simulation model output changes over the response surface of the simulation model. The change in the variance of the mean as the parameters s and d are changed is shown graphically in Figure 44. This plot of simulation output of variances is comparable to the plot in Figure 9a of the simulation output of mean cost. The plot in Figure 44 is based on one observation of the variance of the mean of 10 replications at each of 420 points discussed in Chapter 4. Since the plot in Figure 44 is based on only one observation from the computer simulation at each of the 420 points, it is expected that the surface in Figure 44 is much more irregular than the shape of the true surface of the variance of the mean.

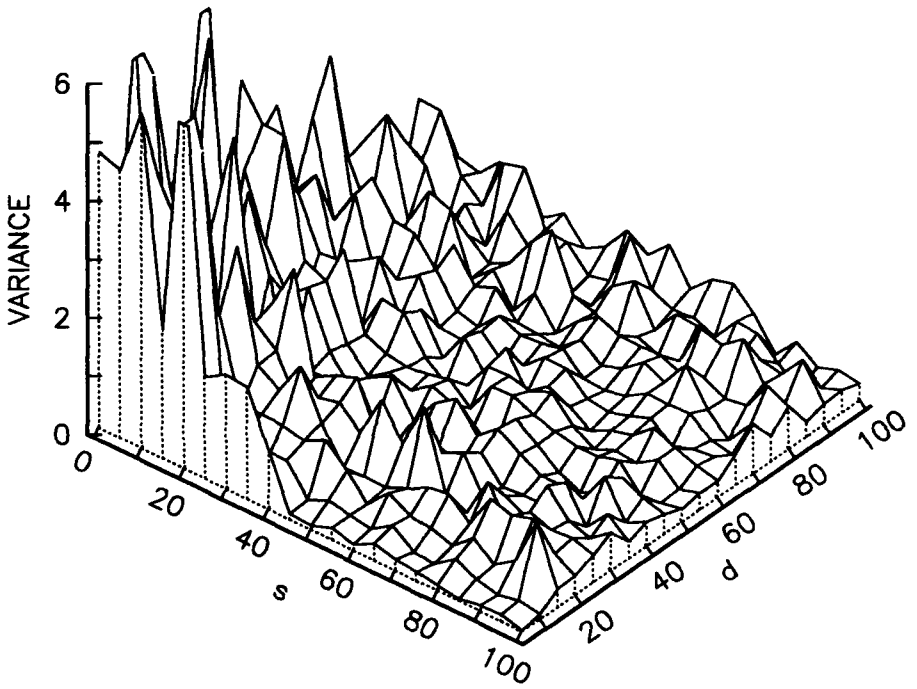


Figure 44 Surface Plot of Variance of Mean Cost Based on Direct Simulation

5.4.1 Examining Four Input Dimension ANN Variance Results on a 2 Dimensional Surface

Figure 45 shows the predictions made by the neural network developed using the individual replications of data set F that correspond to the direct simulation results shown in Figure 44. It should be noted that the variances plotted in Figure 44 are based on 10 replications at the 420 points described in Chapter 4. All of the points had the same values for the parameters k and w. The parameter k was set to 32 and the parameter w was set to 6.4. The closest values in training set F to these settings are with k equal to 16 or 32 and w equal to 8. Also there are only 16 values in the (s,d) space. In spite of the sparseness of the training data and its dissimilarity with the test set the plot of predicted values for the ANN trained on the individual replications of training set F appears to mimic the surface of the simulation response.

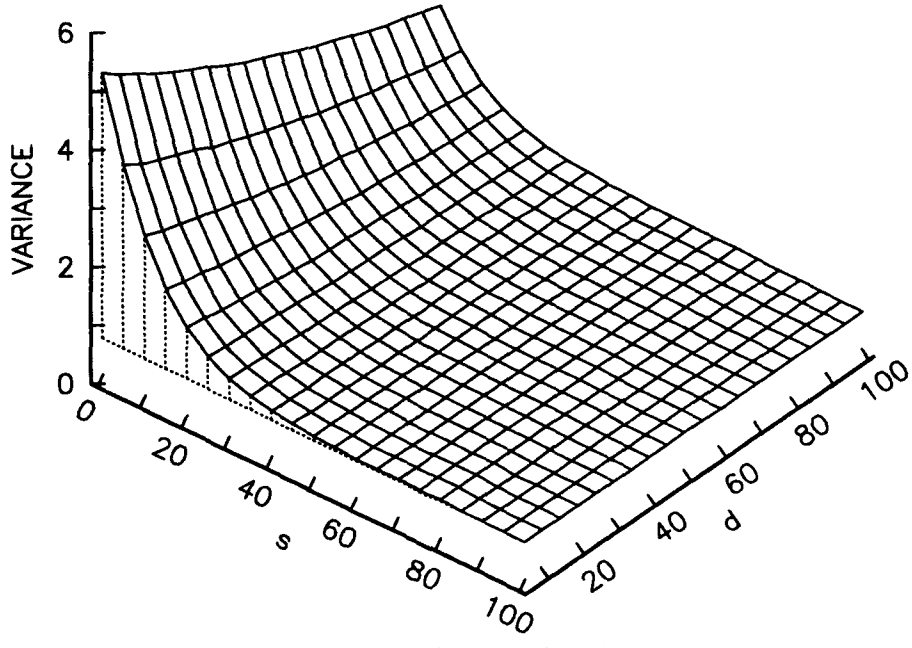


Figure 45 ANN Predictions of Variance using Training Set F

5.4.2 Results of Experiment 5

Separate networks were used to estimate the variance of the expected cost prediction of the computer simulation of the inventory system. The networks had the same architecture and the same training strategy of those in experiment 4. The target output of the simulation was s^2/n as defined in equation 5-2, i.e., the sample variance divided by the number of replications in the set. In this experiment the number of replications used to develop the variance of the mean was 10. Other statistics also could have been used such as the standard error (i.e., square root of the variance of the mean), sample variance (i.e., the number of observations times the variance of the mean), or the sample standard deviation (i.e., the square root of the sample variance). Because the confidence intervals used in analyzing the results of computer simulations are calculated using square root of the variance of the mean, it was appropriate to use it in this research. Since the number of replications used to calculate the variance of the mean was always ten, the interpretation of the networks trained on this data is that tney would estimate the variance of the mean with a sample size of ten.

In experiment 4 networks trained on data sets A, B, C, and D appeared to not have enough data while those trained on data sets E and I appeared to have too much of one type of data. Networks trained on sets F, G, H, J, K, L, and M appeared to do well. To reduce the workload but still be able to consider the advantage of adding additional data points, only three of the training sets were used in succeeding experiments. Data set F was chosen as the smallest data set that realized good performance. Data sets H and K were selected since they added the most information possible to data set F in terms of the input parameters s and d for set H and the input parameters k and w for set K. Examples of the initial networks and the best trained networks are at Figures B6 and B7.

respectively. An example of the data (Set F) used to train the networks on the variance of the mean is shown in Table B3 under the column Var($\overline{C}$). The data used to test the ANN is described in Table 12. The test set values for the variance of the mean were obtained by averaging the variance of the mean of ten different sets of ten replications each. The variance of the mean of each set of ten replications was calculated using equation 5-2. Two of the test sets described in Table 12 are provided in this dissertation. The simulation results for the test set with 0 factors external is at Table B4 under the column Var($\overline{C}$). The simulation results for the test set with 4 factors external is at Table 13 under the column Var($\overline{C}$).

The range of the variance of the mean was from 0.03 to 48.93 with an average value over the 900 points of the entire test set of 1.64. After experimenting with various combinations of distances to extend the scaling range on the outputs, the best combination found was 10% of the range lower than the minimum value and 20% of the range higher than the maximum value.

Each of the networks in this experiment were trained for 750 epochs. The networks were evaluated after each epoch, and the one which performed best on the training set was saved as the final trained network. The number of epochs required to reach the minimum training error for each of the training sets is shown in Table 15. The average number of epochs required to reach the minimum training error was 424 epochs.

The results of training and testing the three networks on the variance of the mean are shown in Table 15. From these results it is apparent that there is not much gained by increasing the number of data points from training set F to either training set H or training

set K. The percentage of the average MAE of the networks trained using these data sets to the mid-range value of the variance of the mean test set is 40% (100*0.66/1.64). This indicates that predicting the variance is a difficult problem. The variance predictions did not suffer much when going from the training set to the testing set, indicating good generalization ability. The results on the various subsets of the test set are shown in Table 16. In addition to the performance of the ANN metamodels, the result of one additional set of ten replications of direct simulation of the test set points are also provided in Tables 15 and 16. As can be seen in Tables 15 and 16, the ANN metamodels typically produced better results than the ten replication of direct simulation. As the number of input parameters that are external to the training set increases, the mean absolute error of the ANN metamodels increase as shown in Table 16. In addition, the mean absolute error of the estimate provided by ten replications of direct simulation on the test points also increases as the number of input parameters increases. This indicates that the variance of the mean is more difficult to predict for the points where the number of external input parameter values is large.

Table 15 Results for Training and Entire Test Sets for Variance Prediction

Training Set	Number of Epochs Until Best Trained ANN	Training MAE	Entire Test Set MAE (900 pts)
F	545	0.46	0.67
H	648	0.61	0.65
K	79	0.53	0.66
Average	424	0.53	0.66
Direct Simulation 10 Replications	-	-	0.80

Table 16 MAE Results for Test Subsets for Variance Prediction

Training Set	Test Set Number of Factors External				
	0	1	2	3	4
F	0.23	0.40	0.71	1.67	2.63
H	0.15	0.32	0.69	1.89	2.66
K	0.25	0.35	0.79	1.67	1.73
Average	0.21	0.35	0.73	1.75	2.34
Direct Simulation of 10 Replications	0.27	0.44	0.76	1.43	9.63

For comparing the difficulty of developing metamodels of the mean to developing metamodels of the variance of the mean, the results for predicting the cost with the same training sets that were used to predict the variance of the mean are shown in Table 17. As can be seen by comparing the results from Table 15 and 17 there is much more variability between the MAE of the different ANN metamodels for predicting cost than for predicting variance. While the size of the error is larger for predicting cost than for predicting variance the percentage of the error to the average value in the test set is much smaller for the cost metamodels than for the variance of the mean metamodels. The average MAE of the networks trained using these data sets to the average value of the cost test set is 5.31% (100*8.45/159). The results for the subsets of the test set shown in Table 18 indicate that the direct simulation of ten replications does better than the ANN metamodels especially as the number of external parameters in the test set increase. This reinforces the previous observations that ANN metamodels perform interpolation fairly well but may not extrapolate very well.

Table 17 Results for Training and Entire Test Sets for Cost Prediction

Training Set	Presentation Method	Number of Epochs Until Best Trained ANN	Training Set MAE	Entire Test Set MAE (900 pts)
F	**PM 1 Averages**	152	6.61	11.59
F	**PM 4 Replications**	58	3.97	6.51
H	**PM 1 Averages**	73	5.59	11.03
H	**PM 4 Replications**	240	3.66	6.66
K	**PM 1 Averages**	340	2.80	6.41
K	**PM 4 Replications**	11	4.78	8.49
Average	-	145.7	4.57	8.45
Direct Simulation	**10 Replications**	-	-	0.86

Table 18 MAE Results for Test Subsets for Cost Prediction

Training Set	Presentation Method	Test Set # of Factors External				
		0	**1**	**2**	**3**	**4**
F	**PM 1 Averages**	4.62	7.37	13.96	22.91	41.83
F	**PM 4 Replications**	2.25	4.04	7.37	14.39	27.02
H	**PM 1 Averages**	6.31	7.22	12.52	21.04	36.54
H	**PM 4 Replications**	1.70	3.69	7.61	15.90	31.71
K	**PM 1 Averages**	1.90	3.48	7.18	15.41	30.35
K	**PM 4 Replications**	2.47	5.37	10.20	18.10	30.99
Average	-	3.21	5.20	9.81	17.96	33.07
Direct Simulation	-	0.72	0.75	0.94	1.14	1.27

5.5 Experiment 6: Comparing Prediction Intervals from Direct Simulation with those Developed from ANN Approximations of the Computer Simulation

To evaluate the overall performance of the neural network metamodels, the neural network estimates of total cost and of the variance of total cost were combined using equation 5-3 to form neural prediction intervals. Prediction intervals are similar to confidence intervals but instead of predicting how often the true mean would fall in an interval they predict how often an observation from the distribution would fall in the interval. While prediction intervals are not used by the simulation community as often as confidence intervals are used, they do provide an efficient means of comparing the accuracy of the intervals developed by the ANN with the intervals developed by direct simulation. The prediction intervals were constructed for each of the 900 test vectors using the neural network predictions for the mean and variance of the mean. In addition similar prediction intervals were constructed directly from 10 additional simulation replications made at each test vector.

$$\text{Prediction Interval} = \overline{C} \pm t_{9,1-\alpha/2} \times \sqrt{\text{Var}(\overline{C}) \text{x} 10} = \overline{C} \pm t_{9,1-\alpha/2} \times s \qquad (5\text{-}3)$$

(Note that s is the estimate of the standard deviation of cost.)

The simulation generated prediction intervals were compared with the neural generated prediction intervals by using 100 additional simulation replications at each test point and counting the number of these which fell into each interval. If the simulation prediction interval or the neural prediction interval were perfect, then a number of replications equal to the confidence level would fall within the interval, with equal numbers falling on either side of the interval. For example, an 90% prediction interval (α= 0.05) should include 90 of the 100 replications with 5 replications falling above the interval and 5 replications falling below the interval, for each test point.

The results for the estimation of the variance of the mean cost for training sets F, H and K are given in Table 14 and the results for the estimation of the mean cost for the same training sets are given in Table 15. While the neural network prediction intervals were not as accurate as those generated by the simulation, in many instances they were quite reasonable. The goodness of the prediction intervals was more dependent on the quality of the neural prediction of total cost, than that of the prediction of variance for this problem. The networks which did poorly for estimation of total cost, also made poor prediction intervals, as might be expected. In general, these were the networks trained on mean value, rather than individual replications. Therefore, it is critical that the networks estimating both the mean value of the simulation and the variance be validated and verified as strongly as possible, before proceeding to building prediction intervals. Table 19 shows the results of the 100 replications averaged over the 144 points of the interpolative test set (no external values) for 90%, 95% and 99% confidence levels.

Table 19 Prediction Interval Results for Test Set 0

Train	Conf.	ANN - Replications			Neural Nets - Mean			Simulation Intervals		
Set	Level	Low	Interval	High	Low	Interval	High	Low	Interval	High
F	90	1.4	83.0	15.6	39.9	57.4	2.7	5.6	88.9	5.5
F	95	0.4	91.3	8.3	29.3	69.5	1.2	2.7	94.3	3.0
F	99	0.0	98.9	1.1	10.8	89.1	0.1	0.6	98.8	0.7
H	90	4.6	82.3	13.1	64.0	33.8	2.2	5.6	88.9	5.5
H	95	2.1	90.6	7.3	55.8	43.0	1.2	2.7	94.3	3.0
H	99	0.2	98.6	1.2	34.6	65.2	0.2	0.6	98.8	0.7
K	90	12.1	83.2	4.7	3.0	89.2	7.8	5.6	88.9	5.5
K	95	6.0	91.5	2.5	1.2	95.6	3.2	2.7	94.3	3.0
K	99	0.7	99.0	0.3	0.1	99.7	0.2	0.6	98.8	0.7

Two further observations from Table 19 can be made. First, the neural network intervals are not likely to be correctly centered. That is, they are biased upwards or downwards. Since the prediction intervals themselves are symmetric, this is an effect of

the prediction of the total cost estimate being too high or too low. Second, the neural network prediction intervals improve as the confidence level increases (and the interval widens). This happens because the estimates of the neural network for total cost, while not always accurate, are close to the target. As the interval widens, the neural network metamodel becomes very similar to the simulation itself for constructing interval estimates.

To examine the effect of extrapolation, Table 20 shows the results of training set F where the network was trained on individual replications. Test sets 0 through 4 results are shown for the network and for the simulation prediction interval at a 95% confidence level. Of course, since the simulation is generated directly, there is no extrapolation. However, the neural network estimates monotonically suffer as more extrapolation is required. This highlights the danger of using metamodels for extrapolation, especially when more than one parameter is being extrapolated. Similar results were obtained for training sets H and K.

Table 20 95% Prediction Interval Results for Training Set F (Replications)

Test Set	Neural Nets - Replications			Simulation Intervals		
	Low	Interval	High	Low	Interval	High
0	0.4	91.3	8.3	2.7	94.3	3.0
1	3.0	81.0	16.0	2.6	93.5	3.8
2	7.2	67.3	25.5	3.1	93.9	3.1
3	13.3	51.4	35.3	2.8	93.5	3.7
4	18.3	37.3	44.0	1.8	94.9	3.4
All	5.5	73.7	20.7	2.8	93.8	3.4

5.6 Synopsis of Conclusions from Experiments 3 through 6

It has been shown that a combined expected value/variance neural network metamodel approach can be successful for establishing prediction intervals of discrete event simulations. For this problem, training on the individual replications yielded more precise predictions of expected values at the expense of longer training times (the size of the training set for replications is ten times the size of the training set for means). It probably would be possible to improve the variance metamodel by using sets of replications for estimating the variance at each point; i.e., instead of a single estimate of variance based on ten replications, one could take ten estimates based on 100 replications (10 sets of 10). This approach would be considerably more expensive in terms of training data requirements. Another approach that would not require as much training data is the technique used in cross validation with test sets. As an example, generate 11 observations and form all 11 possible subsets of size ten. Then determine the variance of each subset and take the average value of the 11 variances of the subsets and use the average value of the variances as the training data. A third approach would be to use more than one sample size when developing the variance of the mean estimates. For example, generate 10 observations, and form all possible subsets of size 2, 3, 4,...,10. Calculate the sample variance of the mean for each of the subsets and then determine the average variance of the mean for all subsets of the same size. If the average variance of the mean is similar regardless of how many observations are in the sample, then use all of the data with the original input parameters. If the average variance of the mean is quite different as one changes the size of the sample, then the ANN would require an additional input, the size of the sample used to calculate the variance of the mean. While this study was promising clearly more work needs to be done on the trade-offs of precision and computational effort when using neural networks as simulation metamodels.

In most cases the networks trained on averages performed much worse than their replication counterparts. One conjecture as to why this happens is the effect of extreme values. The calculated mean of the ten replications gives equal probability mass (0.10) to each replication. A replication representing an extreme outcome will strongly influence the mean. The neural network does not necessarily mimic mean value behavior. Gradient descent (the backpropagation training algorithm) will move to the error surface location which best suits the majority of the observations. The network may find weights which better reflect the true mean by ignoring (or partly ignoring) the extreme replication. Certainly, replication training gives more information to the network, since none of the simulation data is discarded. In fact it is an open research issue as to what neural networks are attempting to learn when being trained on individual replications. One interesting question to consider is whether networks trained on individual replications are learning the mean, a trimmed mean, or the median.

An additional intriguing idea is to train separate networks to learn the quantiles of simulation output rather than just the mean and variance of the mean. In this way a family of ANN could be used to produce the distribution of the simulation output as opposed to just producing the mean and variance of the simulation output. If it is possible to obtain the distribution of the simulation output then it would be possible to capture the stochastic nature of the simulation. This would be important if one were trying to replace a computationally expensive module in a larger computer simulation in which the stochastic behavior of the module is necessary for interaction with the rest of the larger simulation.

5.7 Summary

Four experiments using a four input parameter version of the (s,S) inventory simulation were examined in this chapter. The experiments included determining the number of hidden nodes to use in predicting the cost of the inventory system, predicting the mean cost of the inventory system, predicting the variance of the mean cost of the inventory system and building prediction intervals for the mean cost of the inventory system. The results of determining the number of hidden nodes shows that there tends to be a pattern to the mean absolute error of the test set as the number of hidden nodes in each of the two hidden layers is increased. The pattern of the test set MAE is that it starts to decrease until hitting a minimum value and then continues to increase. This might initially seem counterintuitive since more learning capability is added to the ANN as the number of hidden nodes is increased and so one might expect the error to continually decrease. While the error for the training set does tend to continue to decrease as the number of hidden nodes is increased the inherent danger in doing so is that the network is memorizing the training set data and then does a poor job at generalizing to points that it has not been trained on. Thus, the result of this experiment shows that with too few hidden nodes the ANN doesn't have enough learning power and that if it has too many hidden nodes the ANN can learn the training data too well in a process typically termed overfitting the data. This result indicates the need to have a procedure for finding the best number of hidden nodes to use in developing an ANN metamodel of a computer simulation.

The remaining experiments show that ANN procedure extends quite easily from two input parameters to four input parameters and as is shown visually is

Section 5.3.1 without much lost in terms of accuracy. Neural network metamodels were built for both the mean cost and the variance of the mean cost. As was observed in Chapter 4, the networks constructed using individual replications typically produce better metamodels than those trained on averages. The ANN metamodels of mean and variance are used to form prediction intervals, which are compared to those formed by direct simulation on the test set.

6.0 BASELINE ANN METAMODEL APPROACH

The ANN approach to approximating discrete event computer simulations, developed as a result of the experiments conducted on the inventory simulation in Chapters 4 and 5, is specified in this chapter. This is a necessary step in this fledgling area of research since there is no one "right" approach to an approximation or estimation problem using ANN.

6.1 Description of the Baseline ANN Metamodel Approach

The baseline ANN metamodel approach has three main phases. These phases are: to decide upon and obtain simulation input and output data; to develop the ANN metamodels; and to evaluate the effectiveness of the ANN metamodels in order to determine whether additional da , needed.

6.1.1 Phase 1 of the Baseline ANN Metamodel Approach

To determine and obtain simulation input and output data, the following steps are carried out in this phase of the metamodel approach. The user of the system should be involved in this phase in as much as the selection of which inputs and outputs are important depends on the user.

1. Identify the outputs of the simulation that are of interest.

2. Determine which controllable and uncontrollable inputs would have an effect on the outputs of interest. Select the inputs to be used in building the metamodel.

3. Determine the minimum and maximum values that are of interest for each selected input.

4. Determine how many values between the minimum and maximum values for each selected input are needed for developing the ANN metamodels. If it is only necessary to establish a linear approximation of the relationship between the input parameter and the output measure, then no additional points other than the minimum and maximum values would be needed. If more complicated approximations are desired (e.g., second-order, third-order or higher) then additional values will have to be included.

5. Identify the values between the minimum and maximum values for each selected input that are needed for testing the ANN metamodels.

6. Calculate the total number of points in the selected input parameter space, for both training and testing the ANN metamodels, by determining the number of possible combinations of input parameter values in the training set and the number of possible combinations of the input parameter values in the testing sets.

7. Determine the desired precision of the outputs.

8. Estimate the number of replications needed to achieve the desired precision for each point in the selected input parameter space.

9. Calculate the total number of replications required to be run on the simulation based on the total number of points in the selected input parameter space and the estimated number of replications required for each point.

10. Estimate the time and computer memory requirements for making the computer simulation runs. If the requirements are unreasonable, then repeat steps 1 through 9 until they are reasonable.

11. Run the simulation to obtain the results for the training and testing sets.

12. Perform post-simulation processing to obtain sample averages and variances for each point in the selected input parameter spaces for each of the desired outputs. This step could be eliminated if comparisons between alternative points are not a requirement and the only information desired is an estimate of the output measures for different input parameter settings.

6.1.2 Phase II of the Baseline ANN Metamodel Approach

ANN metamodels for each of the desired outputs are developed in this phase of the approach. If time, or computing resources are limited, then averages and sample variances should be used as the target output. If accuracy of the metamodel is very important, then the individual replications and sample variances should be used. If the only information desired is an accurate tool for estimating the output measures for various input parameter settings, then the individual replication information should be used. The following steps are performed for each of the different output measures that are to be approximated by a metamodel.

1. Randomize the order of the data in the training set so the different values of the input parameters are spread evenly throughout the file of the training data.

2. Select the minimum and maximum values for scaling the inputs and outputs to the ANN training package. A rule of thumb is to use 10% of the range less than the minimum value of the training and testing sets and 10% of the range more than the maximum value of the training and testing sets. In short, the values used for scaling should be set to $\pm$ 10% beyond the range of the training and testing sets.

3. Select an initial setting for the maximum number of epochs for learning, where an epoch is defined as one pass through the training data. In this research the maximum number of epochs varied from 50 to 5,000. Select the training tolerance small enough to ensure the networks do not terminate prior to reaching the maximum number of runs.

4. Initialize the ANN training architecture as follows:

Input layer having one node for each input parameter.

Two hidden layers each with two nodes. If there is some reason to believe that the relationships in the data are too complex to be learned with only two nodes in each hidden layer then the initial number of hidden nodes could be increased.

Output layer having one node.

5. Perform "best net training" using standard backpropagation with a smoothing factor. Best net training simply means that at the end of each epoch the network is evaluated on the training set and the results of the evaluation are written to a file. If the training is being done on individual replications then the testing could be done on the

average values of the training set to prevent unnecessary computations. At the conclusion of training, the results file is examined to determine at which epoch the smallest mean absolute error (MAE) occurred for the training set. Training to this epoch results in the "best trained net." Compare the number of epochs to the "best trained net" to the maximum number of epochs training termination criterion. If the two numbers are close, then the network might benefit from additional training and so the maximum number of epochs should be increased and this step should be repeated.

6. Increase the number of nodes in each hidden layer by one and return to Step 5. Stop this process when no improvement is observed in the test set over previous iterations. If the test set is very small, an alternative is to stop the process when no improvement is observed over previous iterations of a weighted average of the training and test sets mean absolute error.

7. Retrain the initial network in a "learning only" mode, (i.e., no data is written to results files) until reaching the "best trained net" epoch at which time it is saved as the "best trained net." This step is necessary because the weights after each epoch are not stored. This step is much faster than the "learn and evaluate" portion of the training conducted in Step 5.

6.1.3 Phase III of the Baseline ANN Metamodel Approach

To evaluate effectiveness of the ANN metamodels and to determine if additional training data is needed, the following steps are taken in this phase for each of the different output measures.

1. Evaluate the resulting networks in terms of mean absolute error and maximum absolute error for the training and testing sets. If any of these measures exceed the desired performance, then additional training data will be required in order to make the ANN model attain the desired accuracy.

2. Construct confidence intervals and/or prediction intervals using the prediction for the mean and the prediction for the variance of the mean. The validity of the prediction intervals can be checked by obtaining additional independent observations from the simulation and observing the number of observations that fall to the left, inside, or to the right of the prediction intervals.

3. Conduct non-parametric tests on the ranked observations of the simulation data compared to the ANN predictions for both the training and testing sets. If the ANN metamodels do not perform well in comparison to the direct simulation then additional training data will be required.

6.2 Assumptions of the Baseline ANN Metamodel Approach

There are several assumptions that were made in developing the ANN approach to approximating stochastic discrete event computer simulations. These assumptions are listed below:

1. The simulation to be estimated is a terminating simulation.

2. The input parameters of interest are known.

3. The region of the input parameter space over which predictions of the simulation are desired is known.

4. The simulation output measures of interest are known.

5. The simulation output measures being approximated are end of run measures for terminating simulations. In other words, the ANN developed using this approach do not attempt to mimic the behavior of the simulation as it operates over time. The ANN metamodels attempt to predict the end state of the simulation with regard to a particular output measure.

6. The precision with which the ANN approximation of the simulation output is needed is known.

7. The variances of the simulation output are not necessarily equal.

8. The simulation output is a symmetric random variable.

6.3 Limitations of the Baseline ANN Metamodel Approach

The limitations of the baseline ANN approach to approximating discrete event computer simulations are discussed below:

1. The output provided by the ANN developed using this approach are deterministic and cannot be used directly to produce stochastic results.

2. In the regression approach to metamodeling it is possible to characterize the accuracy of the regression estimate through confidence and prediction intervals. Characterizing the accuracy of an ANN estimate for a particular input parameter setting is not possible using this basic approach.

3. The metamodels developed using this approach only provide an estimate of the variance at one particular number of replications of the computer simulation. If increased accuracy is desired then the approach would have to be repeated with an increased number of simulation replications. If an estimate of the variance for a different number of simulation replications is desired then the approach would have to be repeated for that particular number of simulation replications.

6.4 Justification of the Baseline ANN Metamodel Approach

The baseline ANN metamodel approach for discrete event computer simulations was developed as a result of the experiments conducted on the inventory simulation in Chapters 4 and 5. As such it is a first step in developing ANN approximation approaches for computer simulations. Only the major elements of the approach are discussed here since the rationale for the approach is discussed in Chapters 4 and 5.

The method of "best net training" described in Phase II is a variant of "stopped training" which has been described as one of the true innovations to result from neural network research.[139] The purpose of such non-convergent methods is to develop a model with good generalization performance rather than to converge on a truly optimal solution for the training data. Many alternative variations of the approach could have been

used but it is important for the sake of future research to establish a benchmark for comparison purposes.

The reason that a systematic heuristic approach for determining the number of hidden nodes is used is that there is no known algorithm for determining the optimal number of hidden nodes to use in an ANN. If too few nodes are used then the performance of the network is poor due to an inability to capture the training information. If too many nodes are used then the danger exists that the network will just memorize the training data and therefore not do well at generalizing to previously unseen data.

6.5 Summary

The baseline ANN metamodel approach to approximating discrete event computer simulations is described in this chapter. The three phases of the baseline ANN metamodel approach are presented in detail. The first phase of the approach is to determine which simulation input and output data is of interest, estimate the number of replications to obtaining training and testing data, and then running the computer to obtain the simulati data. The second phase of the approach is to develop the ANN metamodels for each of the desired outputs. The steps for setting up the initial architecture, for performing best net training, for determining how many hidden nodes in each hidden layer should be used, and for obtaining the weights for the final ANN metamodel are discussed in the second phase of the approach. The final phase of the baseline ANN metamodel approach is to evaluate the accuracy of the metamodel to determine if it is a satisfactory representation of the computer simulation and ultimately of the actual system being simulated. The assumptions, limitations and justification of the baseline ANN metamodel approach are also discussed.

7.0 DEMONSTRATION PROBLEM - AN EMERGENCY DEPARTMENT (ED) SYSTEM

The ANN approach described in Chapter 6 is applied to a large complex system to demonstrate its applicability to real world problems and situations. Due to the complex dynamics and interactions of inputs, activities and outputs of a typical hospital emergency department (ED), some researchers and practitioners have turned to discrete event stochastic simulation as a tool for examining the emergency room system. A simulation allows various schedule, layout, staffing, procedure and equipment alterations to be tried so that optimal control strategies for the ED can be developed without disrupting vital care providing services. Previous work in simulating the emergency department includes Weissberg [140] and Saunders, Makens and Leblanc.[141]

7.1 Description of the ED System

The emergency department on which the simulation work in this chapter is based is a 750 bed medical center in Pittsburgh, Pennsylvania. The hospital offers comprehensive medical and surgical services and the emergency department services over 4,200 patients per month. The computer simulation used in this dissertation was built by a team of students and faculty from the Industrial Engineering department of the University of Pittsburgh.

7.2 Computer Simulation of ED System

The emergency department simulation used in this research is based on the emergency department of a large teaching hospital in Pittsburgh, Pennsylvania. The

emergency department is modeled with the SIMAN simulation language on an IBM PC machine. The simulation is contained in two parts: the "model frame" and the "experiment frame". The model frame contains all the basic constructs used to represent the actual ED system. Patient related services and locations in the ED are represented in the model frame in separate sections called stations. These stations include such areas as registration, triage, treatment rooms, x-ray, etc. Building the simulation model frame in this modular manner allows the simulation to be more easily verified and validated, and if necessary, to be modified or expanded. The experiment frame contains data such as arrival times, service times, and patient flow patterns as well as the constructs for obtaining output data from the simulation. As a result the user can perform different experiments with the simulation without actually changing the structure of the system as represented in the model frame. The data related changes for the input parameters of the simulation are made only to the experimental frame.

The simulation consists of the following: the ED physical facilities and layout, servers (e.g., physicians and nurses), patients, and procedures for representing patient arrivals, patient activities and treatments, server shift changes and server breaks. The simulation is operated for a 24 hour warm-up period, beginning at 7:30 in the morning, before statistics are taken for the second 24 hour period at which time the replication of the simulation is terminated. Since the emergency department nearly empties out at this time it is appropriate to use the terminating simulation approach for this situation. In order to make development of simulation of the ED tractable, certain simplifying, but realistic, assumptions were necessary. These assumptions along with the simulation constructs are discussed below.

7.2.1 Physical Layout of the ED

The physical locations of the ED consist of 18 treatment rooms (two of which have two beds while the rest have one bed each), a waiting room, a registration desk, a triage room, an x-ray area, and separate stations for the unit secretary, nurses, nurses aides and physicians. The distances and corresponding transit times between each of the locations in the ED are explicitly represented in the computer simulation.

7.2.2 Patient Representation in the ED

Patients are represented as entities that flow through the simulation model. Although there are endless types of patients that visit the ED, it is possible to categorize the patients into three modes of arrival - helicopter, ambulance/medic, and walk-in which includes auto, bus, and jitneys. Patient arrival distributions for two hour blocks of time throughout the day were obtained by fitting actual hospital data for a two month period. The proportion of patient arrivals by each mode of arrival is determined by a discrete probability mass function which is fixed for the 24 hour period.

For each arriving patient, an acuity level is assigned: emergent, urgent, or non-urgent. The probability of a patient having a particular acuity level is determined by a fixed discrete probability mass function which depends on the patient's mode of arrival. An additional categorization of patients is the type of care to be provided to the patient: simultaneous care, where service is provided by multiple servers at the same time; sequential care, where the patient is treated by only one server at a time; and observational care, where nurses provide very little medical treatment other than to periodically check the patient's condition. A final categorization is on the basis of patient disposition: left without treatment; treated and released; admitted to intensive care; admitted to general

care; and departed for morgue. Both the type of care provided and patient disposition are determined by a discrete probability distribution based on the acuity level of the patient.

Some patients being admitted to the hospital arrive at the ED rather than the patient admitting area. These direct admit patients (i.e., destination is admittance) regardless of mode of arrival or level of acuity, have their own distinct flow through the ED: they go to registration and either depart the ED immediately and go to the admittance section of the hospital or are put in an ED treatment room, receive observational care and then depart the ED and go to the hospital admittance section.

All patients whose initial destinations are not hospital admittance use the following paths. The flow of helicopter and ambulance patients, from entry to the ED until arrival at the treatment room, is to be assigned a treatment room and a nurse, to be transported to the treatment room, and for the registration clerk to obtain registration information in the treatment room. For walk-in patients, the flow from entry to the ED until arrival at the treatment room depends on the acuity of the patient. If the walk-in patient's acuity level is emergent, then after a short time at the triage station, the patient follows the path described above for helicopter and ambulance patients. If the walk-in patient's acuity level is not emergent then the patient goes to registration and then triage, waits (if necessary) for a treatment room, is assigned a treatment room and a nurse, and finally is transported to the treatment room. Once the patient arrives in the treatment room, the patient flow no longer depends on mode of arrival, but depends on acuity level, x-ray requirements and laboratory requirements.

There are three categories of laboratory and x-ray requirements: none; routine; and extensive. A category of lab requirements and a category of x-ray requirements are assigned to each patient via discrete probability mass functions depending on the patient's acuity level.

After receiving all necessary treatment the patient departs the ED for a destination determined by a discrete probability distribution which depends on the patient's acuity level. However, for the destinations of intensive care and general care, patients have to remain in the ED if a bed is not available. The time for a bed to become available is based on an exponential probability distribution whose mean is determined by the patient's acuity level. A simplified depiction of the flow of patients through the ED is shown in Figure 46.

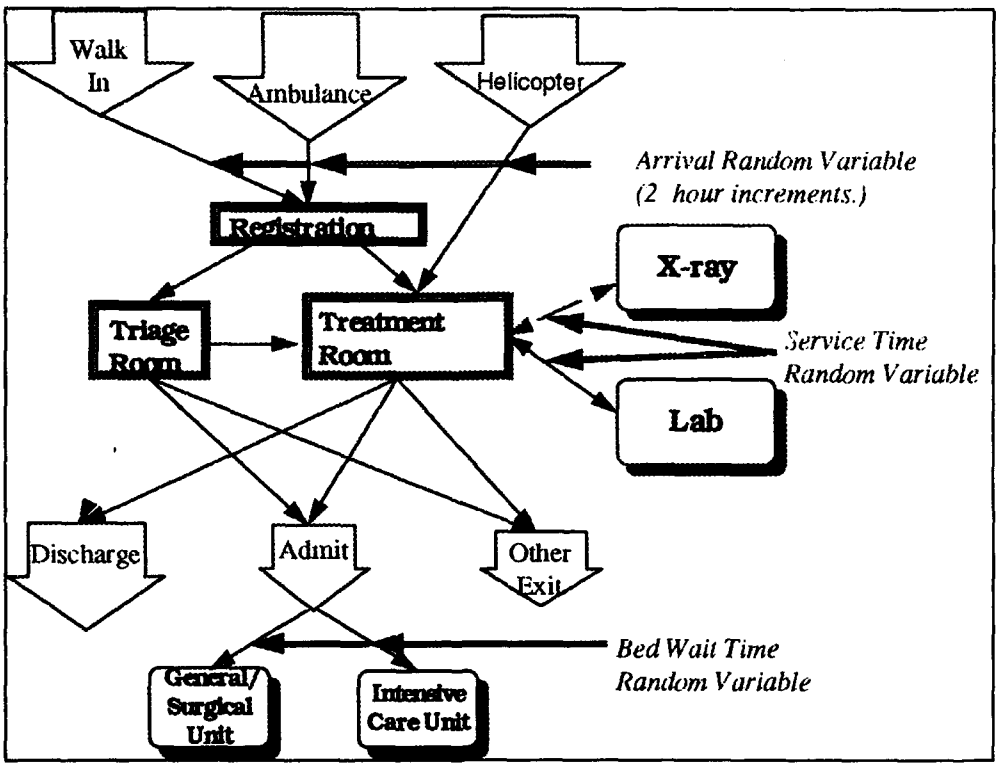


Figure 46 Patient Flow Through the ED

7.2.3 Workers in the ED

The facilities and staff are divided into two categories, those that provide service from a fixed station (e.g., treatment rooms and secretaries) and those that travel throughout the ED (e.g., physicians and nurses). Based on these distinctions, the stationary servers are modeled as resources and the mobile servers are modeled as transporters in the SIMAN simulation. This allows the mobile servers to move freely throughout the ED as well as to transport patients from one location to another. There are three types of physicians: attending; third year residents; and first or second year residents. There are six types of nurses: charge nurse; triage nurse; emergent patient area nurse; urgent patient area nurse; non-urgent patient area nurse and nurses aide. Service times of physicians and nurses and clerks are modeled as exponential distributions with means dependent on the acuity level and care type of the patient. Service times of registration and admittance personnel are modeled as uniform distributions with ranges dependent on arrival mode and acuity level of the patient. Server breaks are combined with lunches to give each worker the unofficial standard 45 minute lunch/dinner break rather than the officially prescribed 30 minute lunch break and two ten minute breaks.

7.2.4 Validation of the Simulation

Using the CINEMA companion to SIMAN, an animation of the ED simulation was developed and shown to hospital personnel to obtain face validation of the computer simulation from the system operators. In addition, output data from the simulation was compared with observed data from the ED system. The quantity of patients and time in the system for different patient categories were extracted from the hospital databases for two months, and estimates were made of mean values. These were compared to the estimates from the simulation model, where the simulation results were the averages of ten

replications of 61, days or two months each. The comparisons are summarized in Table 21. These results show that the computer simulation accurately represents the actual ED.

Table 21 Simulation Comparison with Actual ED Database Records

Patient Type	Number in Database	Number in Simulation	Database Average System Time (Min.)	Simulation Average System Time (Min.)
Emergent	415	451	159	164
Urgent	4091	4166	176	172
Non Urgent	3963	3959	116	123
Total	8469	8576	147	149

7.3 Demonstration of the Baseline ANN Metamodel Approach

In an environment such as the emergency department, where changes in the system occur frequently and with little warning, tactical decisions need to be made quickly. The simulation that was built to examine alternative solutions to problems in the emergency department could not be run quickly enough to provide assistance to the ED management. Thus a neural network metamodel of the ED simulation was constructed to demonstrate the usefulness of the metamodel approach. The following discussion demonstrates the application of the baseline ANN metamodel approach to the ED system.

7.3.1 Phase 1 of the Baseline ANN Metamodel Approach

The first phase of the baseline ANN metamodel approach requires close interaction between the developer of the ANN metamodel and the operator of the system under study. In this case the management of the ED wanted the simulation to be able to provide a reliable estimate of the average time a patient spends in the ED, from arrival until departure. Other simulation outputs of interest to ED personnel included, maximum time

patients spent in the ED, average time patients spent waiting for service, and utilization of rates of the rooms and staff. The ED staff were also interested in the patient related statistics being provided by each acuity type. To keep the demonstration simple, only the most important output of average patient time in the ED was used.

Many different inputs to the simulation were described in Section 7.2. These inputs range from arrival distributions, to percentages of patients of each acuity level, to time to complete various services, to numbers of staff personnel on duty, to the time and duration of staff breaks. The selection of which inputs should be included in the metamodel is guided by the practical application of the metamodel. For this case, the ED staff wanted to understand the effect of changing four specific input variables which were outside of the direct control of the ED personnel but were within the control of other sections of the hospital. The four input parameters of the emergency department simulation examined in this research were the means of an exponential random variable for intensive care bed wait time, general care bed wait time, laboratory service time, and x-ray service time. As was described in Section 7.2, when patients leave the ED they might end up waiting in the ED for a period of time for a bed within the hospital to become available; i.e., either intensive care bed wait time or general care bed wait time.

For each of the input parameters, the initial values of these parameters in the simulation were obtained from a series of regression models of the hospital's actual patient times in the emergency department. The initial values of these parameters were selected as one of the training points for the neural networks. To obtain minimum and maximum values for the variables, each of the parameters was permitted to take on values that were $\pm 100\%$ of the initial settings in the simulation. While additional values could have been

selected for developing the ANN metamodel of the computer simulation, the three values per input parameter are enough to examine the relationship between the input variables and the output measure. Since each of the four parameters had three possible values, the total number of points in the training set was 81 data points. The plot of the training points for each of the pairwise combinations of input parameters is shown in Figure 47. The actual values of the input parameters and the response provided by ten replications of the simulation in terms of the mean and the variance of the mean time in the system is provided in Table C1. The mean and the variance of the mean in Table C1 are determined using equations 7-1 and 7-2. The number of replications was selected as ten since this typically produced variances that were relatively small. The data was shuffled in the order that was used to train the ANN.

In order to evaluate the generalization ability of the ANN, 80 test points were selected from the region internal to the training set. The test points from a pairwise comparison viewpoint are shown in Figure 48. The actual values of the input parameters for the test set and the response provided by 100 replications of the simulation are shown in Table C2. The mean and the variance of the mean in Table C1 are determined using equations 7-3 and 7-4. It should be noted that equation 7-3 is actually calculating the mean of ten averages of different sets of ten replications which is the same as calculating the mean of the 100 replications. However, equation 7-4 is the mean of ten variances of different sets of ten replications which is not the same as the variance of 100 replications. The number of replications was chosen as 100 for the dissertation work however, in actual application it would have been adequate to have ten replications for the test set. To provide a comparison of how well direct simulation performs compared to the ANN metamodels, an additional 20 replications were made and split into two groups of ten

replications each. Estimates of the memory requirements and the time to run the simulation for 10 replications of 81 training points and 120 replications of 80 testing points indicated that this was a feasible task.

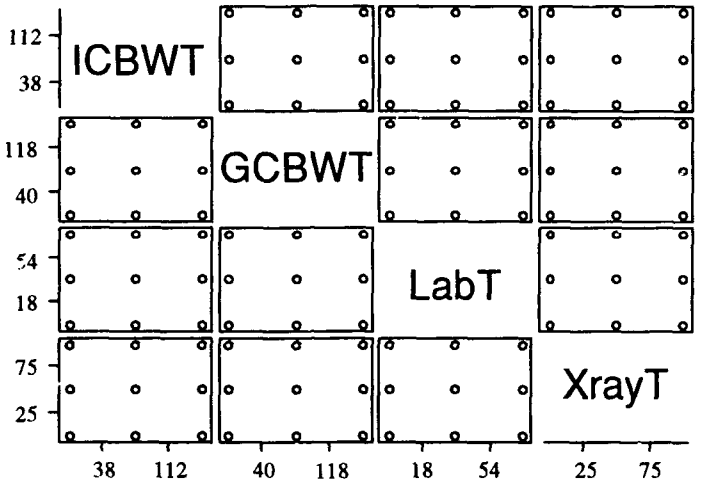


Figure 47 Training Set Values for Emergency Department Simulation

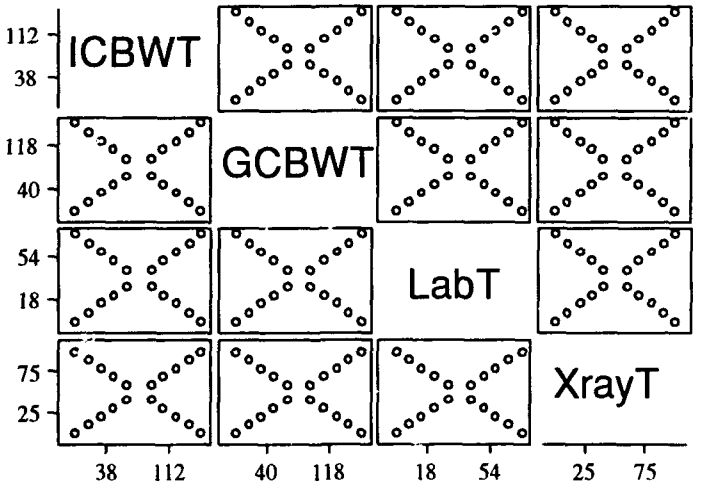


Figure 48 Testing Set Values for Emergency Department Simulation

$$\overline{T}_i = \frac{\sum_{j=1}^{10} T_{ij}}{10} \tag{7-1}$$

$$Var(\overline{T}_i) = \frac{\sum_{j=1}^{10} (T_{ij} - \overline{T}_i)^2}{9 \times 10} \tag{7-2}$$

$$\overline{T} = \frac{\sum_{i=1}^{10} \overline{T}_i}{10} \tag{7-3}$$

$$Var(\overline{T}) = \frac{\sum_{i=1}^{10} \overline{T}_i}{10} \tag{7-4}$$

7.3.2 Phase 2 of the Baseline ANN Metamodel Approach

In this phase, all three types of ANN that could be developed using the Baseline ANN metamodel approach are demonstrated. The first two ANN estimate the average time a patient spends in the emergency department: one using the individual replications and one using the average values of the simulation. The third ANN estimates the variance of the average time a patient spends in the emergency department.

The training data is shuffled to improve the learning process as shown in Table C1. The minimum and maximum values for the output measures used to perform the scaling for ANN training were selected to be ±10% of the range beyond the minimum and maximum values of the training and testing sets, respectively. The training tolerance was set at 0.002 to ensure that the training would not ter reaching the training tolerance. The maximum number of epochs or runs through the training set was initially set at 750. The initial BrainMaker files used for training for the individual replications, averages, and variances are provided in Figures C1, C3 and C5, respectively.

The architecture used for the ANN initially was four input nodes, two hidden layers of two nodes each, and one output node. This network was trained using the "best net training" technique and the best network for two nodes in each hidden layer was evaluated on the test set. Another node was added to each hidden layer and the process was repeated. The number of epochs to reach the best network was compared to the maximum number of epochs permitted. For all three networks the best network was close to the maximum number of epochs. Thus, the maximum number of epochs was increased and training repeated with the maximum number of epochs being 1,000 for the ANN predicting the mean time in the ED and 5,000 for the ANN predicting the variance of the mean time in the ED. For these values of the maximum number of epochs, the networks found their best nets at 870, 259, and 4,853 for the networks trained on individual replications, averages and variances, respectively.

The results for the networks being used to predict mean time in the ED are shown in Figure 49. As can be seen in Figure 49 four hidden nodes per layer results in the lowest MAE on the test set. Ordinarily, the baseline ANN metamodeling approach would have

stopped the search for the best number of nodes in the hidden layers at five nodes since that is where the networks begin to do worse on the test set. For demonstration purposes the process was continued, for selected values out to 22 hidden nodes. As Figure 49 shows, in this case the procedure appears to have selected the best number of hidden nodes. The same process was performed for the network predicting the variance of the mean time in the ED with the result being that the selected number of hidden nodes was seven. The final trained networks for the networks trained on individual replications, averages, and variances are provided in Figures C2, C4 and C6, respectively.

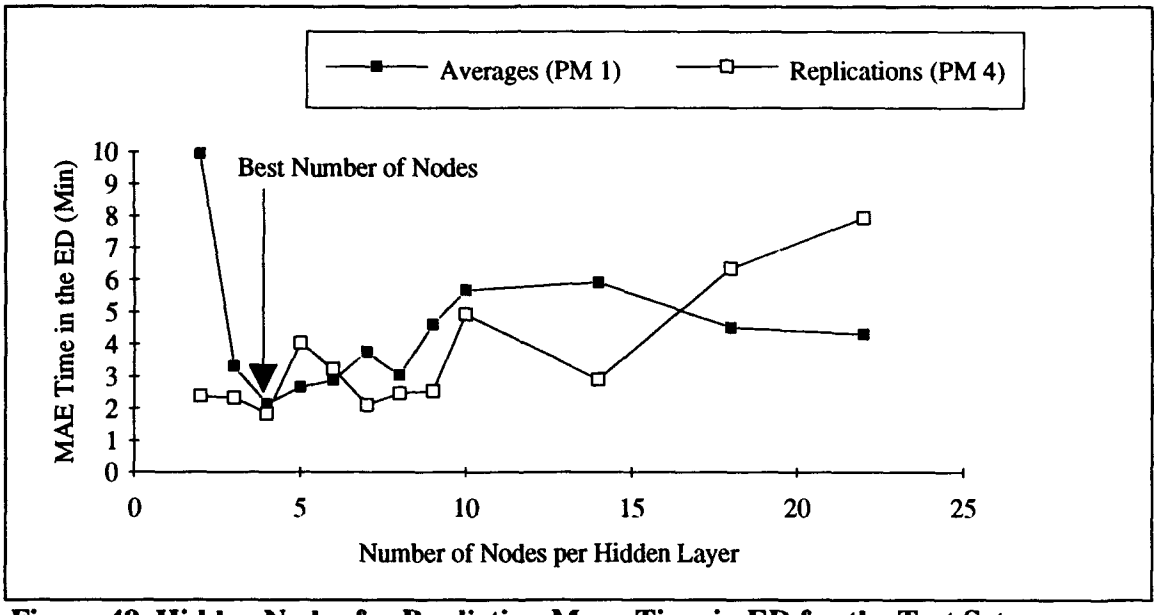


Figure 49 Hidden Nodes for Predicting Mean Time in ED for the Test Set

7.3.3 Phase 3 of the Baseline ANN Metamodel Approach

The results of the ANN training and testing are examined in the third phase of the baseline ANN metamodel approach in order to determine if additional training data is required. The results of testing the ANN for the networks predicting the mean and the networks predicting the variance of the mean are provided in Tables C3 and C4,

respectively. The summary results in terms of mean absolute error and maximum error observed for the each of the ANN compared to the results of 100 replications of the simulation are provide in Tables 22 and 23. Table 22 provides the results for all 80 test points. Table 23 provides the results for 78 of the test points where the points with the two worst errors have been removed. From Table 23 it can be seen that the mean absolute errors of the networks predicting the mean time in the ED, of 2.13 and 1.81, are very low in comparison to the average time in the ED which ranged in value from 115 to 180. The maximum errors of the same networks, 9.4 and 9.2 are also quite small. The results are even more impressive when the two points with the worst testing errors are removed as is shown in Table 23. The results for the variance predictions are not as impressive. While the values for the variance of the test set ranged from 10 to 98, the MAE was 8.6 and the maximum error was 95 as can be seen in Table 22. If the two worst points are removed, the MAE drops to 6.7 and the maximum error drops to a more respectable level of 33.1. This indicates that predicting the variance of the mean is much more difficult than predicting the mean time in the ED.

Also shown in Tables 22 and 23 are the results of using two different sets of direct simulation of the test set, each of size ten replications, to try to predict the "true" answers obtained from direct simulation of 100 replications. Although this would not ordinarily be done in the baseline ANN metamodel approach, the results are instructive. The ANN outperform the ten replication direct simulation in every case except for the maximum error of the variance when considering all 80 test points.

TABLE 22 Comparisons To "True" ED Simulation (100 Replications)

		MAE		Maximum Error	
Estimation Method	**Data Used**	**Mean Time In ED ($\bar{T}$)**	**Var ($\bar{T}$)**	**Mean Time In ED ($\bar{T}$)**	**Var ($\bar{T}$)**
Direct Simulation	Set A - 10 Replications	4.33	14.16	13.03	69.90
Direct Simulation	Set B - 10 Replications	4.22	19.91	11.21	74.80
Direct Simulation	Average MAE of Sets A&B	4.28	17.03	12.12	72.35
ANN	Averages (PM 1)	2.13		9.40	
ANN	Individual Replications (PM 4)	1.81		9.20	
ANN	Variance ($\bar{T}$)		8.6		95.0

TABLE 23 Comparisons To "True" ED Simulation (100 Replications) When Two Worst Errors Are Removed

		MAE		Maximum Error	
Estimation Method	**Data Used**	**Mean Time In ED ($\bar{T}$)**	**Var ($\bar{T}$)**	**Mean Time In ED ($\bar{T}$)**	**Var ($\bar{T}$)**
Direct Simulation	Set A - 10 Replications	4.02	12.42	11.70	61.2
Direct Simulation	Set B - 10 Replications	3.94	11.35	10.40	47.0
Direct Simulation	Average MAE of Sets A&B	3.98	11.88	11.05	54.1
ANN	Averages (PM 1)	1.92		6.80	
ANN	Individual Replications (PM 4)	1.60		4.80	
ANN	Variance ($\bar{T}$)		6.7		33.1

In addition to examining the summary statistics, Figures 50 and 51 provide a visual comparison of the ANN to the "true" answers of 100 replication of computer simulation at the test points. Figures 50a through 50d compare the test set predictions for the network trained on the individual replications for each of the input variables. Figures 50a through 50d all indicate that the ANN are able to closely approximate the mean time in the ED as determined by the computer simulation. Figures 51a through 51d compare the test set predictions for the network trained on the variances for each of the input variables. Figures 51a through 51d indicate that while the variance is a more difficult function to estimate, the ANN does a fairly good job of predicting the variance computer

simulation. Note for the neural network, the test set predictions are an interpolation task, but for direct simulation, the test set is input and replicated as any set of inputs would be.

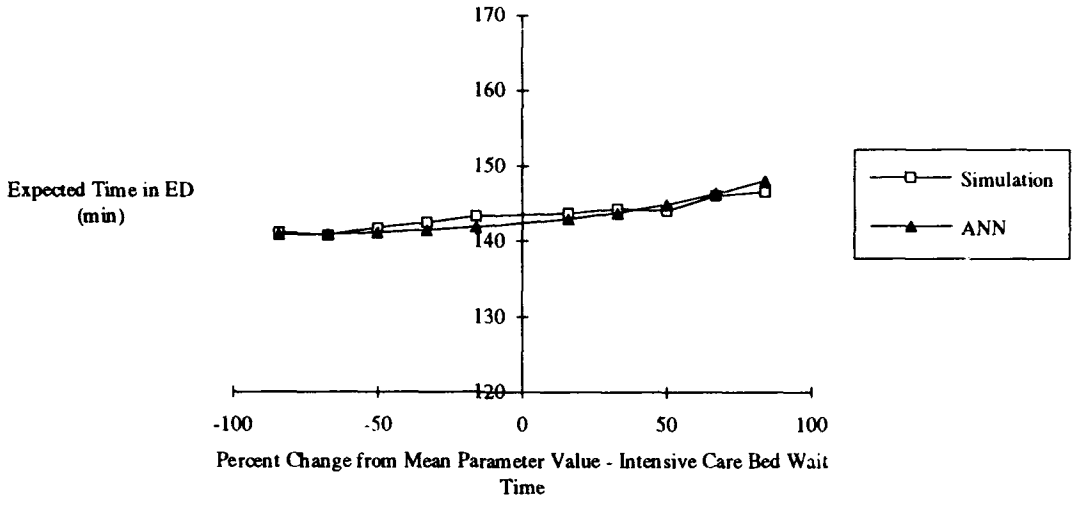


Figure 50a Mean ED Time Results of Neural Network and Simulation for Test Set

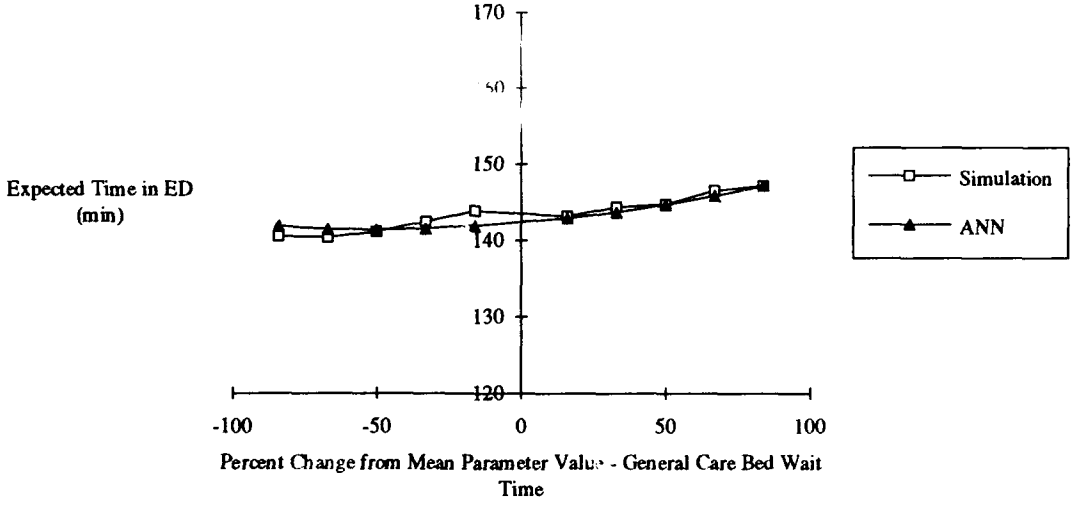


Figure 50b Mean ED Time Results of Neural Network and Simulation for Test Set

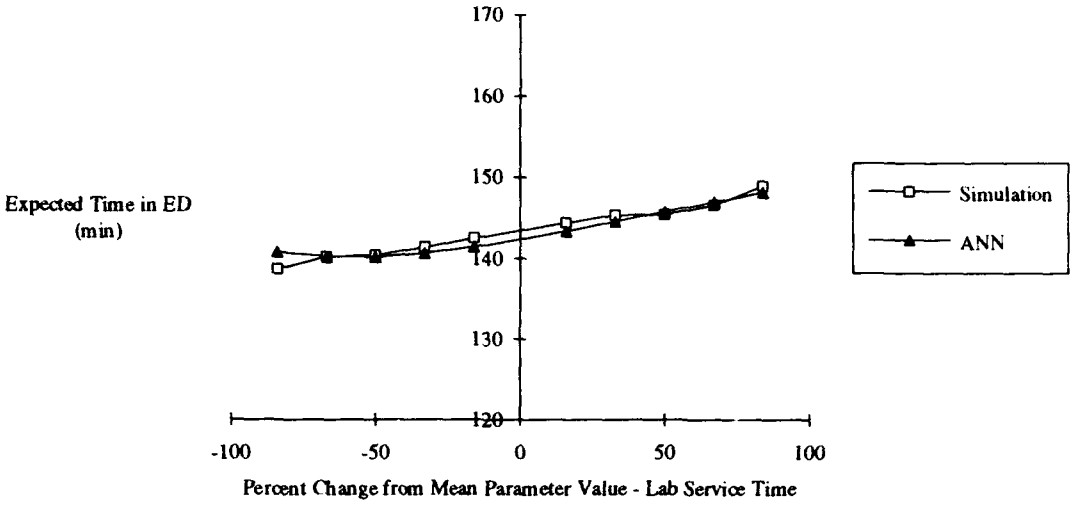


Figure 50c Mean ED Time Results of Neural Network and Simulation for Test Set

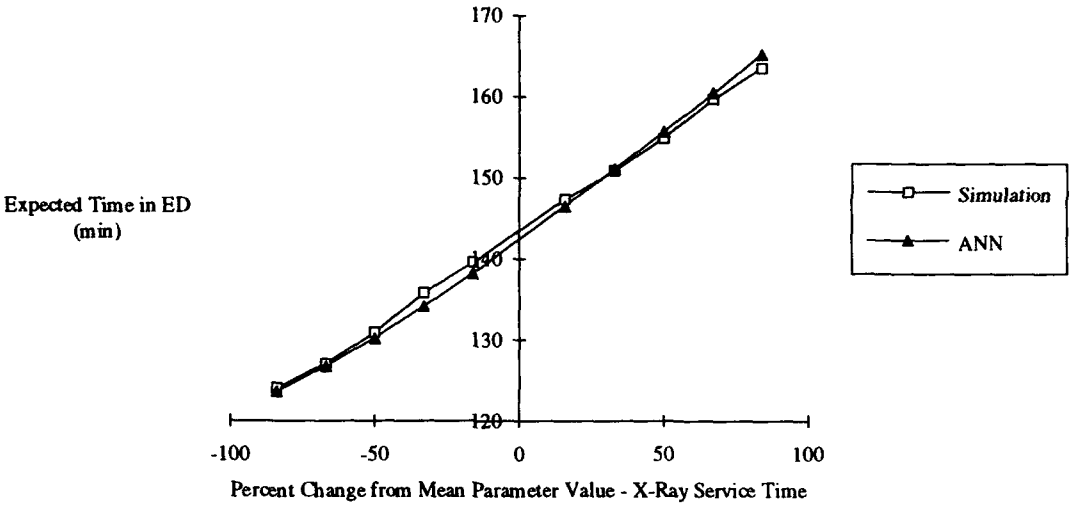


Figure 50d Mean ED Time Results of Neural Network and Simulation for Test Set

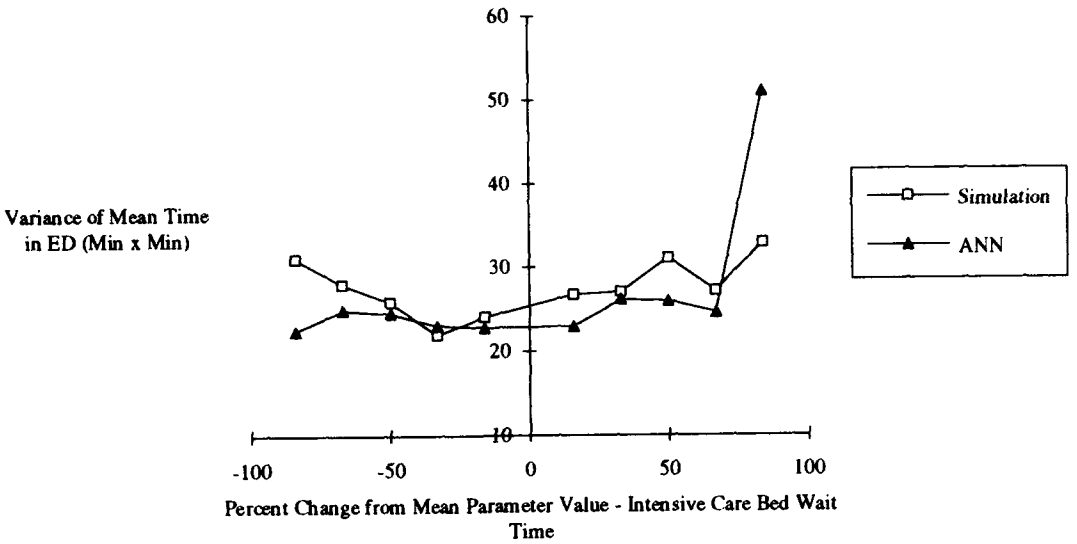


Figure 51a Variance Results of Neural Network and Simulation for Test Set

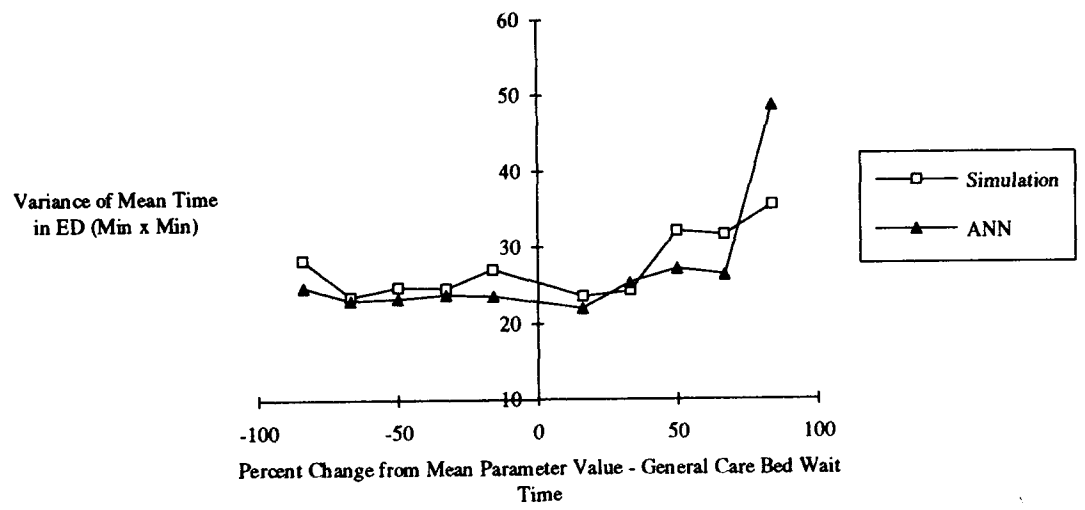


Figure 51b Variance Results of Neural Network and Simulation for Test Set

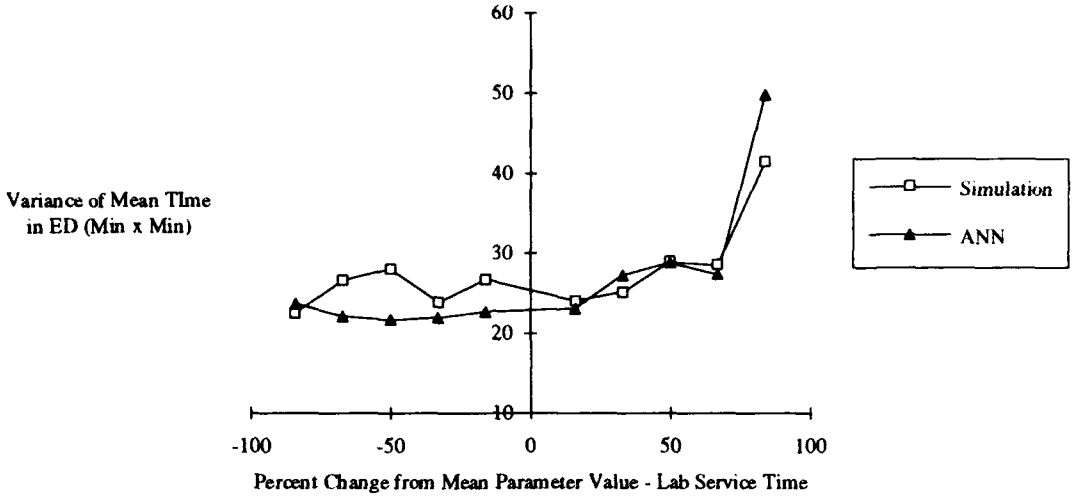


Figure 51c Variance Results of Neural Network and Simulation for Test Set

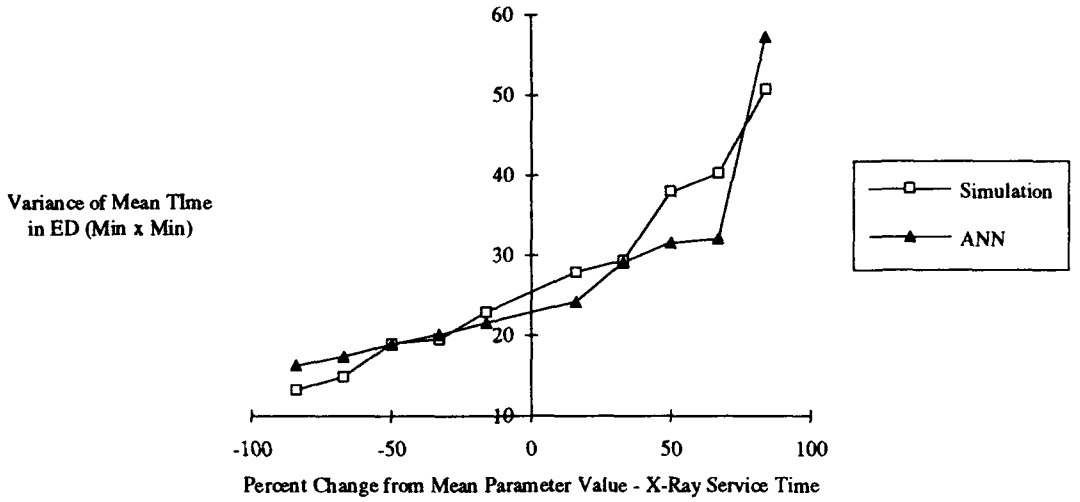


Figure 51d Variance Results of Neural Network and Simulation for Test Set

One of the primary uses of simulation is the development of confidence intervals for the output variables. A comparison of the intervals generated through the neural network metamodel and by direct simulation is a fundamental test of the functionality of the metamodel approach. Confidence intervals are used to estimate the

range within which one expects the mean to fall. In regression, prediction intervals are used to estimate the range within which an individual observation would be expected to fall. In the simulation and statistics fields tolerance intervals are used rather than prediction intervals since the mean and variance are unknown. In regression the mean and variance are assumed to be known when in fact they are not truly known.

Since ANN are also metamodels of the computer simulation, it is appropriate to use prediction intervals for ANN. For comparison purposes prediction intervals are also constructed in this research for the computer simulation output. Prediction intervals for confidence factors of 80%, 90%, 95% and 99% were generated for the test set using the first set of ten extra replications of the simulation and the two parallel neural metamodels (one for expected time and the other for variance). Table 24 shows the comparison of these intervals by the number of 100 separate simulation replications which fell within the interval, fell on the low side of the interval and fell on the high side of the interval. Table 24 shows that the neural network was very accurate in terms of the appropriate number of replications falling within the intervals, and the neural network trained on individual replications was slightly more precise than that trained on means. In fact, for the 80% and 90% intervals the ANN did too well, in that the number falling in the interval was larger than expected. For the 95% and 99% intervals the ANN were closer to the desired levels than the intervals developed using direct simulation data. What this implies is the ANN are too accurate at the 80% and 90% level, to be characterized as being generated by ten replications and that a more appropriate number of replications to enter the t-table for the ANN would be some number larger than ten.

All the intervals in Table 24 do not reflect the symmetry expected in prediction intervals, that is all intervals showed a marked differential in those observations on the high side of the interval versus those on the low side of the interval. An examination of the simulation output from those 100 replications show a positive skewness. This is not unexpected since time in the ED has a definite lower bound in that the time cannot be smaller than zero, but in some cases could be quite long. This highlights the need for research into using the data from the large test set to build empirical e-tables that would be used in the same way the standard t-table is currently used.

Table 24 Prediction Interval Results for Test Set

Conf.	Neural Net - Replications			Neural Net - Mean			Simulation Intervals		
Level	Low	Interval	High	Low	Interval	High	Low	Interval	High
80	5.0	85.9	9.1	4.8	85.8	9.4	8.6	79.2	12.3
90	1.1	93.6	5.3	0.9	93.4	5.7	3.4	88.3	8.3
95	0.2	96.6	3.2	0.2	96.5	3.4	1.4	92.6	6.0
99	0.0	98.8	1.2	0.0	98.7	1.3	0.2	97.2	2.6

The drawback to this procedure is that it still requires the assumption of symmetry of the output data. In cases where the data is asymmetrical it may be possible to construct prediction intervals using order statistics. For instance, instead of training neural networks on the mean and variance which are then used to construct the prediction intervals, it may be possible to train neural networks on the smallest and largest order statistics for each point in the simulation training data. For data with ten replications at each point, the intervals so obtained would be interpreted as 81.82% prediction intervals. (One would expect 1/11 future observations to be smaller than the first order statistic of a sample and 1/11 future observations to be larger than the last order statistic of a sample, if the data

comes from a continuous distribution. This leaves 9/11 future observations to fall between the first and last order statistics.)

On the basis of these results of the summary statistics of MAE and maximum error, the graphical comparison over the range of test set values for each of the input parameters, and the prediction intervals it appears that there is no requirement to obtain additional training data.

7.4 Results of ED System Demonstration

As can be seen from Table 22, the ANN using individual replications performs better than the ANN trained on averages which collaborates the observations from the experiments performed on the inventory simulation. In addition, the ANN metamodels produced better results when trying to predict the "true" mean time in the system and the variance of the mean time in the system than direct simulation of 10 replications. The conclusion to be drawn from these results is that rather than perform direct simulation for various additional combinations of the simulation input parameters, the ANN metamodels could be used to give more accurate estimates of the average patient time in the system without making any additional runs of the computer simulation.

As Figures 50 and 51 indicate, the neural network did extremely well on generalizing its training to the test set. The expected value of time in the system was an easier problem to learn, and therefore predictions are more accurate than for the variance. Variance predictions could probably be improved by training the variance neural network metamodel on sets of replications, i.e., use ten sets, of ten replications each, to develop ten

different variance values for each input vector. This of course would also increase the amount of work to develop the neural network metamodel since 100 replications, instead of ten replications, would be required at each training and testing point.

7.5 Summary

This chapter contains the results of applying the baseline ANN metamodel approach to a demonstration problem. The demonstration problem is based on a computer simulation of an emergency department. The computer simulation is described in terms of the physical layout, flow of patients, and workers in the emergency department. The computer simulation is shown to be a valid representation of the emergency department. The input parameters of concern were the intensive care bed wait time, general care bed wait time, laboratory service time, and X-ray service time. The output measure of interest was the time that patients spent in the emergency department. A total of 81 training points and 80 testing points were selected. The baseline ANN metamodel procedure was followed in developing ANN metamodels of the mean time in the ED using both individual replications and average values. An additional ANN metamodel was constructed to predict the variance of the mean time in the ED. The results of following the baseline ANN training procedure were that the ANN predicting mean time in the ED used four hidden nodes in each of two hidden layers and the ANN predicting the variance of the mean time in the ED used seven hidden nodes in each of two hidden layers. The ANN metamodels as well as two different sets of ten replications of direct simulation of the test set were compared to the "true" response of 100 replications of direct simulation. The results indicated that the ANN metamodels were better predictors than ten replications of direct simulation for both the mean time in the ED and

the variance of the mean time in the ED as shown in Tables 22 and 23.. This should not be taken as a suggestion that the ANN metamodels are performing better than the computer simulation. The only conclusion that should be inferred from these results is that the ANN metamodel appears to be more accurate on the test set than ten replications of the computer simulation. Additionally, the metamodels of the mean time in the ED and the variance of the mean time in the ED were combined to develop prediction intervals. The ANN and direct simulation prediction intervals were both skewed in that more of the 100 observations at each testing point fell to the right than fell to the left of the prediction interval. This observation is not unexpected since time in system data does tend to be skewed to the right since there is a definite lower bound of zero. This observation highlights the need for researching non-parametric methods of constructing confidence and predictions intervals for metamodels. This chapter has demonstrated the application of the baseline ANN metamodel approach and shows how the approach can be beneficial to the simulation of real world systems.

8.0 SUMMARY AND CONCLUSIONS

The baseline ANN metamodel approach to approximating discrete event computer simulations has been demonstrated in this research to be a viable and effective way to develop accurate metamodels of computer simulations.

8.1 The Baseline ANN Metamodel Approach

The experiments discussed in Chapters 4 and 5 on the inventory computer simulation were used to develop and refine the baseline ANN metamodel approach. The specific steps entailed in the approach are provided in detail in Chapter 6. The baseline approach involves using a backpropagation trained artificial neural network to learn the relationship between the simulation inputs and output. The approach consists of three phases. The first phase is to determine what simulation information is of interest in terms of the inputs and outputs of the simulation, to estimate the time required to obtain the simulation information and to obtain the information by running the computer simulation. Training and testing data are obtained from the first phase. The second phase is to develop a neural network approximation of the computer simulation using the data obtained from the first phase as training examples to be learned by a backpropagation trained, full connected, feedforward artificial neural network. The specific form of training that is used is called "best net training." The third phase is to evaluate the results of the trained ANN to determine if additional simulation data is required. The baseline ANN metamodel approach was applied to a large emergency department simulation and the results are provided in Chapter 7 to demonstrate the application of the approach on a real world problem.

8.2 The Performance of the Baseline ANN Metamodel Approach

The results of the (s,S) inventory development problem showed that in terms of accuracy ANN metamodels outperform regression metamodels of the type typically used in response surface methods. The results of this research also show that it is better to use separate networks for different outputs than to have a combined network. In addition, it was shown that networks trained on the individual replication output data had better generalization performance than networks trained on just the averages of the simulation output. As was shown in Chapter 7, the baseline ANN metamodel approach can do well at approximating a computer simulation. In fact, for the demonstration problem, the ANN metamodel trained on 81 data points each with ten replications was able to outperform direct simulation of ten replications on 80 additional test points which were not included in the training set.

It must be noted that neural networks and the other metamodeling techniques commonly used are deterministic. The stochastic aspect of the simulation is lost, however, the metamodel is much faster in operation than the simulation. Therefore, while possibly losing precision when moving from the simulation to a metamodel, the user also loses the rich stochastic framework of the simulation. Surrogates for the stochastic elements, such as expected value, moments and percentiles, must be used in deterministic metamodels. Thus the tradeoffs involve imprecision and simplification for increased speed.

One disadvantage of the ANN metamodel is that it is even more of a "black box" than the original computer simulation. While sensitivity analysis can be performed using the ANN metamodel, it does not have the advantage of the convenient interpretation of the coefficients found in regression metamodels.

8.3 Major Contributions of the Dissertation

The major contribution of this dissertation is the development of a baseline approach for developing ANN metamodels of computer simulations. This baseline approach can be used by other researchers for comparison purposes when developing their own ANN metamodel approaches. This contribution was needed in the field of artificial neural networks because there are many different existing and emerging ANN procedures for performing approximation and estimation tasks. Another specific contribution is the determination that it is best when approximating stochastic computer simulations to use the "noisy" individual replications rather than the "quiet" average values. While the results of this research indicate that ANN are appropriate for use as metamodels of stochastic computer simulations, this research has identified many areas that require additional work and experimentation to take proper advantage of ANN as metamodels.

8.4 Future Research Directions

There are many new research issues that have arisen as a result of the experiments and work performed for this dissertation. The major areas of future research work are divided into three categories: improvements on the baseline ANN metamodel approach, extensions of the approach, and specific applications or uses of the approach.

8.4.1 Improvements of the Baseline ANN Metamodel Approach

A major area of research is in experimental design for neural networks as metamodels of computer simulations. The need for research into experimental design

considerations exists for all types of metamodels.[142] The most critical need is for designs that take into consideration both the development (i.e., training) and the evaluation (i.e., testing and validation) of metamodels. This becomes even more critical if the metamodels are to be constructed using a training set for adjusting the weights and one test set for determining when to stop training and a second test set for evaluation of the generalization ability of the metamodel. Work should build on the research performed using traditional designs from statistics and response surface methods and also those proposed by Taguchi.

A new procedure that could improve the performance of the ANN metamodel approach is ensemble networks.[143] The basic idea is to build several different networks and take the average of their output in order to build a more robust overall network metamodel. This procedure was examined briefly in this research, but is not reported in this document due to it being outside the scope of this research. One idea that was considered in the work supporting this research was to combine the outputs of the networks trained on the different subsets of the training set discussed in Chapters 4 and 5. Other approaches could be to train different networks on different training parameters, on different initial weights, or on different orderings of the training data.

Another area of potential research where success has been achieved with regression metamodels used in RSM is the use of common random numbers and other variance reduction techniques. In this research, all of the simulation data was generated as independent observations for both the training and testing data.

Other research is needed to examine various iterative approaches for developing improvements beyond the baseline ANN metamodeling approach. For instance, it might

make more efficient use of the computer simulation to start with small training and testing sets, in terms of replications, and build ANN metamodels to use in performing factor screening to eliminate those input factors that do not appear to make much of a difference on the simulation output. After eliminating the irrelevant factors the baseline approach could be used on the remaining factors with a substantial savings in total computer simulation runs. Another issue that could be addressed using iterative methods, is to determine what steps should be taken, if any, after developing an ANN and evaluating it on the test set, to improve the ANN. Possible steps would include determining the regions of the input space where the ANN is performing poorly and then deciding on the appropriate corrective action such as obtaining more data points for training or more replications for data points already in the training set.

Research is also needed on the use of extreme values observed from the simulation. For instance in the hospital simulation one of the average output values for a particular combination of the input training parameters, was much larger than all of the other average output values. The research issue would be to determine if such values should be included in the training set.

Another research issue that needs to be examined is a comparison between the confidence intervals obtained using metamodels of the mean and variance versus the confidence intervals obtained using metamodels derived from the lower and upper confidence limits of each point in the input parameter training space as was done in Hurrion's work.[76]

Finally, another major area for future research is examining faster training procedures and alternative types of neural networks that have been developed since the introduction of backpropagation. Networks such as RPROP and radial basis function (RBF) networks are two such candidates.

8.4.2 Extensions of the Baseline ANN Metamodel Approach

One area of research interest is to extend the application of the baseline ANN metamodel approach to predictions over time as opposed to terminal values or values averaged over the length of the simulation run.

A second extension of the ANN approximation approach is to model non-terminating simulations. Some of the new approaches such as infinitesimal perturbation analysis which use one long single run of the simulation rather than many replications may be a useful way to obtain data for training a neural network metamodel of a simulation.

A third area for future extensions of the baseline ANN metamodel is to develop empirical confidence and prediction intervals rather than intervals based on the Normal or t-tables.

One of the drawbacks of the approach developed in this research is that it transforms a stochastic computer simulation into a deterministic ANN metamodel. In some applications, such as modules within a very large computer simulation, the stochastic nature of the module is essential to the proper operation of the computer simulation. Thus, another area of research is to build a family of ANN that would attempt to capture more than just the mean and variance of the output of the simulation. This family of ANN

would have n members, one for each of the n replications, and each member would be trained on just one of the order statistics for all points in the input training space. In this way the entire cumulative distribution function for each point in the input parameter space could be estimated. Using this estimated cumulative distribution function and the inverse transform method it would be possible to replace a large module in a computer simulation with a stochastic rather than a deterministic approximation. This is an important consideration since models are being used to do more than analysis. Simulation models are being used for training in industry and to support large scale exercises in the military. Future generations of such simulations which will incorporate advanced features such as virtual reality will also need ways of aggregating models that are appropriately stochastic.(144)

8.4.3 Applications of the Baseline ANN Metamodel Approach

One application of ANN metamodels that needs additional research is in response surface methods. Based on the work in this research ANN trained for a very short time, say only a few epochs, may very well provide an adequate estimate to perform response surface optimization. Response surface methods estimate the shape of the response surface in a small region and move away from that region toward improvement in the measure of interest. Additional data is then gathered to estimate the surface in the new region and the process is repeated until there is evidence that an optimum has been reached. Based on the results of this research which found the errors of the training and testing sets decreasing rapidly after one or two epochs it may be possible for ANN to replace first-order regressions in finding the direction of improvement in response surface methods. However, first-order regressions have the advantage of knowing the direction of improvement by just calculating the derivative of the first-order regression equation. A

more suitable use of ANN in traditional RSM would probably be as a replacement to the second-order regressions which are used to determine if the RSM procedure has reached the optimum and should terminate. In this portion of the RSM procedure, accuracy is more important than speed. The results of this research have shown ANN metamodels can be more accurate than second- order regression metamodels and therefore have the potential for improving the termination portion of response surface methods. Additional research is needed that compares ANN and regression metamodels in traditional response surface methods.

Another area of research is the application of using neural networks trained on computer simulations to "feed" non-gradient based optimization procedures such as genetic algorithms and simulated annealing. In these approaches, the only thing needed by the optimization procedure is an objective function or "fitness function" that informs the optimization procedure of the value of the output measure or the "fitness" of a particular combination of the input parameters.[145] In these types of optimization procedures, the added information of the direction of improvement in first-order regression models is of no benefit. The fitness function could be the direct simulation, however, that could cause the optimization procedure to be very slow.

An alternative is to use a metamodel of the simulation as the fitness function. The metamodel would need to be more global in nature than the metamodels used in traditional response surface methods. In traditional RSM, the search begins at one random point and slowly moves along successive approximations of the response surface towards the optimum. In a genetic algorithm based procedure, the search would begin at many different points and find promising areas that would warrant additional investigation.

After finding the most promising areas, it might be necessary to obtain additional simulation runs to develop more accurate metamodels in the most promising areas. Thus, the genetic algorithm approach would proceed from crude metamodels of a very large region to increasingly accurate metamodels in smaller regions of the response surface. Research into non-gradient based optimization procedures using ANN metamodels to optimize computer simulation is needed to determine if such approaches would be competitive with the traditional response surface methods.

In situations where limited system data is available, research efforts are needed to explore ways of using that information in concert with computer simulation to improve the validity of ANN metamodels. One simple approach is to adjust the results of the computer simulation based on ANN trained on real system data. Suppose a small set of input and output data, set A, is available for both the real system and the computer simulation. Train two different ANN: one on set A_r, from the real system and one on set A_c, from the computer simulation. Additional data is obtained from the computer simulation on a much larger data set B with each input point x having an average output of y(x). Since the computer simulation may be a biased model of the true system, the computer simulation results from data set B are adjusted using the neural networks developed on the smaller data set A on the real system data and on the simulation data. One adjustment of the output value of y(x) for each input point x of data set B that could be made is shown in equation 8-1. The simulation data adjusted to be closer to the real system data would then be used to train a third neural network. Such an approach could be used to keep large computer simulations from being rebuilt every time there is a change in the system. In addition, this type of approach could also be used as a procedure for validating new computer simulations of existing systems.

$$\text{Adjusted } y = y \times \frac{\text{ANN Trained on Real System Data (x)}}{\text{ANN Trained on Computer Simulation Data (x)}} \qquad (8\text{-}1)$$

One final application of metamodels created with the baseline ANN metamodel approach that requires additional research is as on-line process controllers. In this capacity the ANN are trained off-line using computer simulations and then are used on-line to assist in the control of the process. In addition, the ANN metamodels could continue to be improved and adjusted off-line as additional real system data and computer simulation data becomes available. The conceptual approach presented by Wan and Cochran should be applied and examined.[92]

8.5 SUMMARY

The ANN approach to approximating discrete event computer simulations has been shown to be an effective way of developing accurate metamodels of computer simulations. The results of experiments on a development problem of a simple simulation led to the baseline ANN metamodel approach. The approach was used on a computer simulation of a real system to clearly demonstrate the approach and its resulting benefits to the simulation community. This chapter summarizes the baseline ANN metamodel approach, the results of applying the approach, the contributions of the dissertation and the specific suggestions for additional research in improving the baseline ANN metamodel approach, for extending the approach to handle different types of problems, and for areas in which the approach has application potential.

APPENDIX A

APPENDIX A

DEVELOPMENT PROBLEM 2 PARAMETER INVENTORY SIMULATION COMPUTER PROGRAMS AND RESULTS

```
BEGIN;
PROJECT,       inv2par;
;  The number of distinct training data points is 36.
;  Total number of replications is  REP x 36= 360.
;
VARIABLES: GET:          !Determine which input point to read.
           REP,10:       !REP = # reps to run each data point.
           SmallS:       !s = reorder point.
           SmallD:       !d = order quantity, if I = s.
           I,60:         !Inventory level.
           Io:           !Initial inventory level.
           tba,.1:       !Parameter for time between arrivals.
           k,32:         !Fixed portion of monthly order cost.
           u,5:          !Underage cost.
           w:            !Underage factor.
           Z:            !Amount to order this month.
           BigS:         !S = order up-to quantity.
           AvgInvPlus:   !Equals I, if I>0, else it = 0.
           AvgInvMinus:  !Equals -I, if I<0, else it = 0.
           OrderCost:    !Monthly order cost.
           COST:         !Cumulative order cost.
           TotalCost;    !Avg annual total cost.
;
TALLIES:
       1, Order Costs; !Tallies order cost each month.
;
DSTATS:1,I,INVENTORY:  !Keeps track of inventory levels.
       2,1*AvgInvPlus, !Calculates/tracks cost of overage.
       Excess Inv Cost:!
       3,u*AvgInvMinus,!Calculates/tracks cost of shortages.
       Short Inv Cost; !
;
FILES:
 1,INPUT1,"inv2par.IN", DIR(17)     !File to set
 "(F3.0,1X,F3.0)":                  !  input parameters.
 2, OUTPUT1,"inv2par",              !File to receive Write
    SEQ,FREE;                       !  statements.
;
REPLICATE, 360,0,120;               !Number of replications.
END;
```

Figure A1 SIMAN Experiment Frame of 2 Input Parameter Inventory System

```
 BEGIN, No,inv2par;
;This is the model frame for the 2 input parameter inventory problem.
;The inputs to the simulation are s (reorder point) and d (reorder qty).
;In this model k(order costs) and w (factor representing ;u, underage
cost) are constanst with k=32 and w=6.4.
;The simulation output is average monthly cost, C.
;This uses 3 different Random Number Streams.
;This section obtains the input data at the beginning of each
;replication.  This assumes that each data point is run for Rep # of
;replications.
;
CREATE,    1,0:,1;                      !Do once for each rep.
ASSIGN:    GET=1+AINT((NREP-1)/REP);    !Determines which input data to use.
;                                       !Every REP replications get next
;                                       !  data point.
READ,      INPUT1,                      !Gets data from file
  "(F3.0,1X,F3.0,1X,F3.0,1X,F5.1)",     !  labeled, INPUT1.
  GET:SmallS,SmallD,k,w;                !SmallS=s=reorder point
;                                       !SmallD=d=order quantity
ASSIGN:    BigS=SmallS + SmallD:        !BigS=order to quantity.
           u=k/w;
DELAY:     0:
           DISPOSE;
;
;
CREATE,   ,EXPONENTIAL(tba,1):          !Arrivals of demands.
           EXPONENTIAL(tba,1);          !Random Stream#1 = 1
BRANCH,    1,4:                         !Levels of demand.
;                                       !Random Stream#2 = 4
           WITH,.167,d1:                !Demand is 1.
           WITH,.333,d2:                !Demand is 2.
           WITH,.333,d3:                !Demand is 3.
           WITH,.167,d4;                !Demand is 4.
d1 ASSIGN:I = I - 1:                    !Demand set to 1.
           NEXT(d5);
d2 ASSIGN:I = I - 2:                    !Demand set to 2.
           NEXT(d5);
d3 ASSIGN:I = I - 3:                    !Demand set to 3.
           NEXT(d5);
d4 ASSIGN:I = I - 4:                    !Demand set to 4.
           NEXT(d5);
d5 ASSIGN:AvgInvPlus=MX(0,I):           !AvgInvPlus=I, if I>0,
;                                          else, AvgInvPlus = 0.
           AvgInvMinus=MX(0,-I):        !AvgInvMinus=-I, if I<0,
;                                          else, AvgInvMinus=0.
           DISPOSE;
;
;
CREATE,    ,1.0:1.0;                    !Calculate cost at end
;                                       !  of each month.
ASSIGN:    OrderCost = 0;
BRANCH,    1:
           IF,I.ge.SmallS,cost1:        !If inventory is large
;                                       !  enough, go to cost1.
           ELSE,cost2;                  !If inventory is not
;                                          large enough, go to
;                                          cost2.
```

Figure A2 SIMAN Model Frame of 2 Input Parameter Inventory System

```
cost1      ASSIGN:Z = 0;                !Nothing ordered this month.
           TALLY: 1, OrderCost:
           DISPOSE;
;
cost2      ASSIGN:Z = (BigS-I);         !Order Z amount.
           ASSIGN:OrderCost= k+3*Z;     !Cost spent on orders this month.
           ASSIGN:COST =                !Cumulative cost
                  COST + OrderCost;     !  of orders to date.
           TALLY: 1, OrderCost;
           DELAY: UNIFORM(.5,1.0,8);    !Wait for order arrival.
;                                       !Random Stream#3 = 8


ASSIGN:    I = I + Z:                   !Increase inventory by Z
           AvgInvPlus=MX(0,I):          !AvgInvPlus=I, if I>0, ;
;                                       !  else AvgInvPlus = 0.
           AvgInvMinus=MX(0,-I):        !AvgInvMinus=-I, if I<0,
;                                       !  else AvgInvMinus = 0.
           DISPOSE;
;
;
CREATE,    ,120:1,1;                    !After 10 year period,
ASSIGN:    TotalCost=                   !  calculate average
           TAVG(1)+DAVG(2)+DAVG(3);     !  monthly total cost as
;                                       !  the sum of average ;
;                                       !  order,overage &
;                                       !  underage costs.

WRITE,     OUTPUT1,
           "(1X,2(F5.1,1X),F10.5)":
           SmallS, SmallD, TotalCost:
           DISPOSE;
END;
```

Figure A2(Continued) SIMAN Model Frame of 2 Input Parameter Inventory System

```
  0   5
  0  20
  0  40
  0  60
  0  80
  0 100
 20   5
 20  20
 20  40
 20  60
 20  80
 20 100
 40   5
 40  20
 40  40
 40  60
 40  80
 40 100
 60   5
 60  20
 60  40
 60  60
 60  80
 60 100
 80   5
 80  20
 80  40
 80  60
 80  80
 80 100
100   5
100  20
100  40
100  60
100  80
100 100
```

Figure A3 Input Data File for SIMAN Simulation of 2 Input Parameter Inventory System

Table A1 Simulation Results: Training Data for Experiment 1 for Presentation Method 1 with 25 Replications

Simulation Input Parameters		Simulation Output Measure Cost = C
s	d	$\overline{C}$
40	40	125.91
60	40	144.64
40	60	132.39
60	60	151.07
20	20	125.47
80	20	164.69
20	80	127.52
80	80	179.86
40	20	125.96
60	20	144.51
20	40	120.19
80	40	165.12
20	60	122.09
80	60	171.96
40	80	140.59
60	80	159.00

Table A2 Simulation Results: Training Data for Experiment 2 for Presentation Method 1 with 25 Replications

Simulation Input Parameters		Simulation Output Measures Cost = C			
s	d	$\overline{C}$	Std Dev (C)	Min (C)	Max (C)
40	40	125.91	101.33	12.04	299.16
60	40	144.64	103.04	18.24	314.08
40	60	132.39	118.56	13.22	351.55
60	60	151.07	119.12	22.37	371.81
20	20	125.47	67.27	7.19	272.12
80	20	164.69	61.01	44.72	282.73
20	80	127.52	128.05	13.15	406.54
80	80	179.86	134.18	35.42	468.60
40	20	125.96	62.06	12.12	239.90
60	20	144.51	59.97	25.29	259.47
20	40	120.19	94.20	9.00	309.46
80	40	165.12	104.07	33.48	338.61
20	60	122.09	112.52	11.21	353.54
80	60	171.96	120.33	36.89	396.69
40	80	140.59	132.31	14.63	407.56
60	80	159.00	132.45	24.23	420.81

Tab Simulation Results: ANN Testing Data for Experiment 1

Simulation Input Parameters		Simulation Output Measure
s	d	$\overline{C}$
10	10	167.02
50	10	135.32
90	10	174.98
10	50	125.64
90	50	178.11
10	90	130.86
50	90	154.01
90	90	194.29
30	30	119.52
50	30	132.92
70	30	152.42
30	50	122.16
50	50	138.25
70	50	157.96
30	70	128.45
50	70	145.36
70	70	165.47

Table A4 Simulation Results: ANN Testing Data for Experiment 2

Simulation Input Parameters		Simulation Ouptut Measures			
s	d	$\overline{C}$	Std Dev(C)	Min(C)	Max(C)
10	10	167.02	58.95	14.21	337.35
50	10	135.32	28.57	31.14	210.65
90	10	174.98	29.23	70.91	270.68
10	50	125.64	100.64	13.29	352.63
90	50	178.11	112.88	41.14	394.50
10	90	130.86	135.18	16.62	461.30
50	90	154.01	138.99	19.48	445.72
90	90	194.29	140.77	46.63	510.70
30	30	119.52	86.15	9.38	271.21
50	30	132.92	88.40	14.00	276.34
70	30	152.42	88.96	27.81	299.00
30	50	122.16	107.79	11.04	318.12
50	50	138.25	111.45	15.58	330.39
70	50	157.96	112.04	27.96	353.84
30	70	128.45	123.46	12.21	374.61
50	70	145.36	125.74	17.58	387.89
70	70	165.47	126.74	30.87	411.06

```
input number 1 2
output number 1 1
hidden 2 2

filename testfacts nn.tst
filename trainfacts j1a113.fct
filename teststats j1a113.sta

learnrate  1.0000 50  1.0000 75  1.0000 90  1.0000
learnlayer  1.0000  1.0000  1.0000
traintol  0.100  0.1000  0.8000 100
testtol  0.1000
maxruns 5000
smoothing  0.9000  0.9000  0.9000
addhidden sequence 0.1 200

function hidden1 sigmoid  0.0000  1.0000  0.0000 1
function hidden2 sigmoid  0.0000  1.0000  0.0000 1
function output sigmoid  0.0000  1.0000  0.0000 1

dictionary input s d
dictionary output tc
display network progress

scale input minimum
0 5
scale input maximum
100 100
scale output minimum
50
scale output maximum
225
statistics 0 0 0
weights 4 1 2 2 2 1
-1.5510  0.6200  3.0620
 3.1592 -4.5006 -0.3210
 0.3232  5.6954 -6.7302
-1.4922 -1.0282  2.9280

 0.1166  2.5932  0.2082
```

Figure A4 Initial Brainmaker Training File for Experiment 1 for Presentation Method 1 with 25 Replications

```
input number 1 2
output number 1 1
hidden 2 2

filename testfacts nn.tst
filename trainfacts j1a113.fct
filename teststats j1a113.sta

learnrate  1.0000 50  1.0000 75  1.0000 90  1.0000
learnlayer  1.0000  1.0000  1.0000
traintol  0.1000  0.1000  0.8000 100
testtol  0.1000
maxruns 2688
smoothing  0.9000  0.9000  0.9000
addhidden sequence 0.1 200

function hidden1 sigmoid  0.0000  1.0000  0.0000 1
function hidden2 sigmoid  0.0000  1.0000  0.0000 1
function output sigmoid  0.0000  1.0000  0.0000 1

dictionary input s d
dictionary output tc
display network progress

scale input minimum
0 5
scale input maximum
100 100
scale output minimum
50
scale output maximum
225
statistics 2688 863 167
weights 4 1 2 2 2 1
-2.7802 -0.0096  2.0540
 2.4082 -4.9984 -1.2006

 0.3232  5.6954 -6.7302
-2.9304 -0.5290  2.0776

 0.7850  2.3508 -0.9942
```

Figure A5 Trained Brainmaker File for Experiment 1 for Presentation Method 1 with 25 Replications

Table A5 Example Brainmaker Results for Training Data for Experiment 1 for Presentation Method 1 with 25 Replications

Input Parameters		Predicted	Target		Absolute	Squared
s	d	Cost	Cost	Difference	Difference	Difference
40	40	143.2	125.9	-17.3	17.3	299.29
60	40	151.7	144.6	-7.1	7.1	50.41
40	60	144.2	132.3	-11.9	11.9	141.61
60	60	153	151.1	-1.9	1.9	3.61
20	20	135.1	125.4	-9.7	9.7	94.09
80	20	157.9	164.6	6.7	6.7	44.89
20	80	137.3	127.5	-9.8	9.8	96.04
80	80	162.5	179.8	17.3	17.3	299.29
40	20	141.3	125.9	-15.4	15.4	237.16
60	20	149.3	144.5	-4.8	4.8	23.04
20	40	136.4	120.2	-16.2	16.2	262.44
80	40	160.3	165.1	4.8	4.8	23.04
20	60	137	122	-15	15	225
80	60	161.8	171.9	10.1	10.1	102.01
40	80	144.6	140.5	-4.1	4.1	16.81
60	80	153.6	159	5.4	5.4	29.16
				Average	9.84	11.03

Table A6 Example Brainmaker Results for Testing Data for Experiment 1 for Presentation Method 1 with 25 Replications

Input Parameters		Predicted	Target		Absolute	Squared
s	d	Cost	Cost	Difference	Difference	Difference
10	10	131.8	167	35.2	35.2	1239.04
50	10	143.7	135.3	-8.4	8.4	70.56
90	10	161.3	174.9	13.6	13.6	184.96
10	50	134.2	125.6	-8.6	8.6	73.96
90	50	164.9	178.1	13.2	13.2	174.24
10	90	134.6	130.8	-3.8	3.8	14.44
50	90	149	154	5	5	25
90	90	166.6	194.2	27.6	27.6	761.76
30	30	138.9	119.5	-19.4	19.4	376.36
50	30	146.4	132.9	-13.5	13.5	182.25
70	30	154.9	152.4	-2.5	2.5	6.25
30	50	140.1	122.1	-18	18	324
50	50	148	138.2	-9.8	9.8	96.04
70	50	156.9	157.9	1	1	1
30	70	140.5	128.4	-12.1	12.1	146.41
50	70	148.7	145.3	-3.4	3.4	11.56
70	70	157.9	165.5	7.6	7.6	57.76
				Average	11.92	14.84

Table A7 ANN Results for Experiment 1

# of	Patterns Shown	Training Set		External Test		Internal Test		Combined Test	
Replications	Until Trained	mae	rmse	mae	rmse	mae	rmse	mae	rmse
Presentation Method 1 (Train on averages)									
1	2928	7.4	9.5	13.2	17.9	8.5	10.1	10.7	14.3
2	2608	9.1	10.6	13.7	17.7	9.2	10.9	11.3	14.5
3	2512	9.8	11.1	14.2	17.9	9.4	11.1	11.6	14.7
4	2464	9.7	11.1	14.2	17.9	9.2	11	11.6	14.6
5	2512	9.4	10.7	14.2	18.2	8.8	10.5	11.3	14.6
6	2608	9.3	10.6	14	17.9	9	10.7	11.3	14.5
7	2528	9.4	10.8	13.9	17.8	9.1	10.8	11.4	14.5
8	2432	9.7	11.1	14.1	17.9	9.2	10.9	11.5	14.6
9	2416	9.8	11.1	14.4	18	9.4	11.1	11.7	14.8
10	2448	9.8	11.1	14.4	18	9.4	11.2	11.8	14.8
15	2496	9.7	11	14.3	18	9.4	11.1	11.7	14.8
20	2528	9.7	11	14.5	18.1	9.3	11.1	11.7	14.8
25	2688	9.8	11	14.4	17.8	9.7	11.6	11.9	14.8
Presentation Method 2 (Train on averages and all individual replications)									
1	2928	7.4	9.5	13.2	17.9	8.5	10.1	10.7	14.3
2	3168	8.3	10	13	17.6	8.6	10.2	10.7	14.2
3	3264	8.7	10.2	13.1	17.6	8.6	10.2	10.7	14.2
4	3440	8.4	9.8	13.3	18	8.1	9.6	10.5	14.2
5	3744	7.6	9	13.4	18.8	7	8.4	10	14.3
6	4032	7.4	8.8	12.7	18.5	7.1	8.5	9.7	14.1
7	4736	7.4	8.7	12.6	18.2	7.2	8.5	9.7	14
8	4752	7.5	8.8	12.8	18.7	6.9	8.2	9.7	14.1
9	4480	7.6	8.9	12.8	18.4	7.4	8.6	10	14.1
10	5632	7.4	8.7	12.7	18.3	7.3	8.3	9.8	13.9
15	5376	7.4	8.7	12.9	18.5	7.1	8.4	9.8	14.1
20	5824	7.4	8.7	12.8	18.5	7.2	8.4	9.9	14.1
25	13392	5.8	6.9	11.4	18.5	6	7	8.6	13.7
Presentation Method 3 (Train on averages and half of replications closest to the average)									
1	2928	7.4	9.5	13.2	17.9	8.5	10.1	10.7	14.3
2	2848	8.4	10.2	13.1	17.7	8.6	10.3	10.7	14.2
3	2624	9.7	11.1	13.8	17.6	9.4	11.2	11.5	14.6
4	2784	9.3	10.7	13.7	17.6	9.1	10.8	11.2	14.4
5	2784	9.1	10.4	13.8	18.1	8.7	10.3	11.1	14.5
6	2752	8.9	10.3	13.8	18	8.6	10.2	11	14.4
7	2752	9.1	10.4	13.5	17.8	8.8	10.4	11	14.4
8	2800	9.1	10.4	13.9	18.1	8.5	10.1	11	14.4
9	2640	9.4	10.7	14.1	17.9	8.9	10.6	11.3	14.5
10	2592	9.2	10.5	14	18	8.8	10.4	11.2	14.5
15	2496	9.2	10.5	14.3	18.3	8.7	10.4	11.4	14.7
20	2800	8.9	10.2	14.3	18.6	8.3	9.9	11.1	14.6
25	3328	9	10.3	14.4	18.4	8.7	10.2	11.4	14.6

Table A7(Continued) ANN Results for Experiment 1

# of Simulation Replications	Patterns Shown Until Trained	Training Set		External Test Set		Internal Test Set		Combined Test Set	
		mae	rmse	mae	rmse	mae	rmse	mae	rmse
Presentation Method 4 (Train on all individual replications)									
1	2928	7.4	9.5	13.2	17.9	8.5	10.1	10.7	14.3
2	2848	8.4	10.2	13.1	17.7	8.6	10.3	10.7	14.2
3	3168	8.8	10.4	13	17.5	8.8	10.4	10.8	14.2
4	3072	8.6	10.1	13.2	17.8	8.4	9.9	10.6	14.2
5	3680	7.6	9	13.2	18.8	7	8.4	9.9	14.3
6	4128	7.3	8.7	12.8	18.4	7.2	8.5	9.8	14.1
7	3920	7.6	8.9	12.7	18.4	7.2	8.6	9.8	14.1
8	4224	7.6	8.9	12.7	18.5	7.1	8.4	9.7	14.1
9	4464	7.5	8.8	12.8	18.4	7.3	8.4	9.9	14
10	4800	7.6	8.9	12.9	18.5	7.2	8.5	9.9	14.1
15	5104	7.4	8.7	12.7	18.3	7.3	8.4	9.8	13.9
20	5184	7.5	8.8	12.9	18.6	7.2	8.4	9.9	14.1
25	12960	5.8	6.9	11.4	18.5	6	7	8.6	13.7
Presentation Method 5 (Train on half of individual replications nearest to the average)									
1	2928	7.4	9.5	13.2	17.9	8.5	10.1	10.7	14.3
2	2848	8.4	10.2	13.1	17.7	8.6	10.3	10.7	14.2
3	2624	9.7	11.2	13.8	17.5	9.5	11.2	11.5	14.5
4	2624	9.3	10.8	13.7	17.7	9.2	10.9	11.3	14.5
5	2688	9.1	10.5	13.8	18	8.8	10.4	11.1	14.5
6	2976	9	10.4	13.7	17.9	8.8	10.4	11.1	14.5
7	2832	9.1	10.5	13.5	17.7	8.9	10.5	11.1	14.4
8	2688	9.2	10.5	13.7	17.9	8.7	10.4	11.1	14.4
9	2688	9.2	10.5	14	17.9	8.8	10.4	11.2	14.5
10	2400	9.3	10.6	14	17.9	8.9	10.6	11.3	14.5
15	2480	9.2	10.6	14.2	18.1	8.8	10.5	11.3	14.6
20	2784	9.1	10.4	14.2	18.3	8.6	10.3	11.2	14.6
25	3120	8.8	10.1	14.3	18.3	8.6	10.1	11.3	14.5

```
input number 1 2
output number 1 4
hidden 10 10

filename testfacts nn.tst
filename trainfacts k1ma113.fct
filename teststats k1ma113.sta


learnrate  1.0000 50  1.0000 75  1.0000 90  1.0000
learnlayer  1.0000  1.0000  1.0000
traintol  0.1000  0.1000  0.8000 100
testtol  0.1000
maxruns 5000
smoothing  0.9000  0.9000  0.9000
addhidden sequence 0.1 200


function hidden1 sigmoid  0.0000  1.0000  0.0000 1
function hidden2 sigmoid  0.0000  1.0000  0.0000 1
function output sigmoid  0.0000  1.0000  0.0000 1

dictionary input s d

dictionary output tc dev min max


display network progress

scale input minimum
0 5
scale input maximum
100 100
scale output minimum
55.0 25.0 0.0 106.0
scale output maximum
281.0 211.0 89.0 813.0
```

Figure A6 Initial Brainmaker Training File for Experiment 2 for Presentation Method 1 with 25 Replications

```
statistics 0 0 0
weights 4 1 2 10 10 4
-5.0486  2.2434 -3.0836
 1.3206 -0.0520 -2.0980
-2.7300  1.1026  1.6966
 2.2674  2.6892 -4.4440
-4.4172 -1.5036 -3.6222
 0.3994  1.6960  6.0102
-5.0910 -1.6560  4.2352
 5.4370  2.0584 -3.1956
 3.4502  2.1282  0.1236
 1.9454 -4.5570 -2.7208

 0.9874  0.7010 -0.9702  1.2382  0.8206 -0.7154 -0.3380 -0.6474 -1.1070 -3.5036  0.0232
 0.6122  1.4126 -2.5616 -1.5422  1.4970  0.3614  0.5196  0.1796  3.8596 -0.8794  1.9872
-0.8006  1.3508  0.4114  0.4420 -2.0914  0.5342 -1.2392 -1.6560  1.0524 -0.2264  1.5990
 2.0206 -2.3522 -0.2120 -0.8800  0.5544  1.6720  2.1454  0.4494  1.9700  0.8230 -1.2886
 2.0004 -1.4472 -1.2832  0.2836 -1.9874 -1.4870 -0.1832  0.4236 -2.8570 -1.1520 -2.6220
-0.4296 -0.1454 -1.0852 -2.4404  2.0194 -1.5880 -1.0892  2.8494  0.8626 -2.0160  1.3964
-0.0006  0.5876 -2.9450 -0.7756  2.2360 -1.0062  2.4906 -1.8470 -0.4832 -2.2580  0.9036
 0.2686  0.7316 -2.1646 -0.6510 -2.0454  0.5508 -0.3816  1.2086  1.0220  2.0226 -1.7508
 0.1600  2.0396 -1.5036 -1.2152  1.2796  3.4722 -0.7574 -1.9202 -0.0592  1.0932  0.8092
 1.3770 -1.6050 -0.9394 -2.4152 -0.3066  1.2474  3.8882 -1.6362 -0.0340  1.8940  0.3260

 2.2424  2.4424  0.6054  1.1072  1.6270 -2.3304 -3.0034  0.2164  3.3362 -0.3492  0.5716
 0.0210 -0.0344  0.6262  0.5802  0.7216 -1.4782 -0.2860 -0.8212  0.3552  0.8330 -0.1046
-0.6280  2.3244  0.5300  0.4770  0.4890 -2.6820  1.1336  0.1064 -1.8132 -0.5210  0.9874
-0.2144  1.0280 -1.8250  0.7846  1.3650 -1.1714  1.7096  0.5652  0.0054 -1.1694 -3.3736
```

Figure A6(Continued) Initial Brainmaker Training File for Experiment 2 for Presentation Method 1 with 25 Replications

```
input number 1 2
output number 1 4
hidden 10 10

filename trainfacts k1ma113.fct
filename testfacts nn.tst
filename teststats k1ma113.sta


learnrate 1.0000 50 1.0000 75 1.0000 90 1.0000
learnlayer 1.0000 1.0000 1.0000
traintol 0.1000 0.1000 0.8000 100
testtol 0.1000
maxruns 2?40
smoothing 0.9000 0.9000 0.9000
addhidden sequence 0.1 200


function hidden1 sigmoid 0.0000 1.0000 0.0000 1
function hidden2 sigmoid 0.0000 1.0000 0.0000 1
function output sigmoid 0.0000 1.0000 0.0000 1

dictionary input s d

dictionary output tc dev min max


display network progress

scale input minimum
0 5
scale input maximum
100 100
scale output minimum
55 25 0 106
scale output maximum
281 211 89 813
```

Figure A7 Trained Brainmaker File for Experiment 2 for Presentation Method 1 with 25 Replications

```
statistics 2240 1547 139
weights 4 1 2 10 10 4
-5.2680  2.8024 -3.7534
 1.1550 -0.7332 -2.2190
-3.1484  1.3264  1.4234
 2.1908  3.0162 -3.7854
-5.0694 -0.8594 -4.0312
 0.2292  2.1124  6.2640
-4.9640 -1.7240  4.1696
 5.4650  2.4524 -2.2600
 3.8614  2.3420  1.1880
 1.7192 -4.9576 -3.6284

 0.9874  0.2812 -1.0364  0.8224  0.8206 -1.6860 -0.1796 -1.4716 -2.0776 -3.5036 -0.9496
 0.6122  1.3882 -2.7472 -1.3710  1.4970 -0.0796  0.0936  0.0970  3.5150 -0.8794  1.5420
-0.8006  1.3634 -0.0970  0.0784 -2.0914  0.3366 -1.5524 -1.6170  0.9102 -0.0260  1.3862
 2.0206 -2.1420  0.1002 -0.3916  0.5544  1.9814  2.1012  0.5266  2.2802  0.8230 -0.9652
 2.0004 -1.4504 -1.0554  0.7234 -1.9874 -1.8086 -0.2666  0.5562 -3.1470 -1.1520 -2.9424
 0.2164  0.1384 -0.3286 -2.5166  2.0194 -0.6892 -0.2504  2.8940  1.5186 -1.3682  2.3100
 0.2212  0.6874 -2.9064 -0.7200  2.2360 -0.6990  2.5396 -1.6910 -0.1942 -2.4212  1.1720
 0.2686  1.0542 -2.6706 -0.9172 -2.0454  0.7136 -0.4692  1.3474  1.1602  2.2346 -1.5594
 0.1560  1.8596 -0.9346 -0.9466  1.2796  3.5140 -0.3954 -2.0462  0.0002  0.5172  0.8844
 1.3770 -1.6244 -1.3452 -2.7112 -0.3066  0.9056  3.6504 -1.8450 -0.4022  1.4774 -0.0272

 2.0104  1.5194 -0.1836  0.1990  1.6270 -3.1066 -2.3566  0.1806  2.6470 -0.5656 -0.3566
 0.0362  0.3522  0.8252  0.9316  0.7216 -0.7906 -1.8386 -1.6984 -0.5964 -0.4344  0.3282
-0.4496  2.0892  0.3264  0.1256  0.4890 -2.6370  1.0610  1.5546 -1.7660 -1.3060  0.5934
-0.0084  1.8710 -1.0764  1.6994  1.3650 -0.2510  0.7236 -0.5572 -0.1712 -1.4162 -2.3592
```

Figure A7(Continued) Brainmaker Trained File for Experiment 2 for Presentation Method 1 with 25 Replications

Table A8 ANN Results for Experiment 2 on the Training Set

# of Simulation Replications	Patterns Shown Until Trained	Mean Cost		Standard Deviation		Minimum Cost		Maximum Cost	
		mae	rmse	mae	rmse	mae	rmse	mae	rmse
Presentation Method 1 (Train on Averages)									
1	20816	6.4	9.2	3.8	26.9	7.3	10.6	4.9	32.8
2	2272	6.5	12.8	4.7	37.1	8.7	13.1	5.4	43.9
3	2784	10.9	12.4	3.9	34	12.5	12.8	4.6	41.9
4	2528	6.3	13.3	4.2	35.3	8.7	13.6	5	43
5	2160	10.5	14.2	4.4	35.5	11.9	14.6	5.2	43.8
6	2272	6.4	12.2	4.6	35.3	7.5	12.6	5.3	43.5
7	2304	11.2	14.1	4.6	36	12.6	14.5	5.3	44.3
8	2288	4	12.5	4.7	35.8	6.1	13	5.5	44.2
9	2160	8.9	14	5.1	36.6	10.2	14.6	5.8	44.3
10	2096	11.3	12.9	5.3	36.3	13.2	13.4	5.9	44.8
15	2336	12	11.6	4.7	35.1	13.7	12.3	5.5	43.6
20	2048	8.9	13.8	5	34.9	10.3	14.1	5.7	42.9
25	2240	8.6	14.2	4.7	35.9	9.6	14.5	5.5	43.7
Presentation Method 2 (Train on averages and all individual replications)									
1	20816	6.4	9.2	3.8	26.9	7.3	10.6	4.9	32.8
2	40320	5.7	7.5	4	38.7	7.7	9.1	4.9	42.3
3	320064	4.6	5.8	3.8	19.2	5.7	7.2	4.8	24.1
4	400080	6.3	3.2	3.8	23.3	7.2	4	4.8	27.4
5	480096	3.4	4.8	4	24.5	4.2	5.5	4.9	27.9
6	560112	8.4	8.5	3.8	17.8	9.5	9.1	4.7	23.9
7	640128	3.4	5.1	3.6	15.4	4.1	6.3	4.5	19.8
8	720144	7.7	3.8	4.1	24.4	8.4	4.5	5	28.9
9	800160	5.3	6.3	3.6	45.6	6.4	8.1	4.6	49.5
10	880176	7.2	3	3.8	27.9	8.5	3.9	4.8	32.1
15	960192	7.2	4.8	4	25.1	8.8	6.1	5	28.8
20	1040208	8.2	8.5	4.4	29.7	9	9.5	5.6	33.7
25	2480496	10.5	11.7	8.1	24.6	14.7	14.4	10.1	29.5
Presentation Method 3 (Train on averages & half of replications nearest average)									
1	20816	6.4	9.2	3.8	26.9	7.3	10.6	4.9	32.8
2	20096	4.5	8.4	4.5	36.8	5.8	9.7	5.4	40.6
3	10336	5.4	7.8	4.1	37	7	9.1	5	40.1
4	240048	9	8.4	4.1	34.6	9.9	9.1	4.8	38.9
5	13200	5	8.9	4.4	28.3	5.7	10.2	5.3	32.3
6	31680	6.6	7.7	4.2	26	8	8.6	5	30.9
7	9536	7.4	7.5	3.8	26.6	9.3	8.5	4.7	31.4
8	27120	10.4	8.1	3.4	24.4	12.1	9.3	4.3	28.3
9	32480	9.4	9.1	3.4	18.2	10.9	10.1	4.2	22.9
10	19392	7	6.6	3.7	25.8	8.7	8.1	4.6	30.7
15	55680	9.7	6.9	3.3	19.1	11.2	8.2	4	23.3
20	560112	10.8	4.2	3.3	20.1	11.6	4.9	4.1	24.5
25	1280256	3.5	7.4	4.7	20.2	4.2	8.6	6.1	25.9

Table A8(Continued) ANN Results for Experiment 2 on the Training Set

# of Simulation Replications	Patterns Shown Until Trained	Mean Cost		Standard Deviation		Minimum Cost		Maximum Cost	
		mae	rmse	mae	rmse	mae	rmse	mae	rmse
Presentation Method 4 (Train on all individual replications)									
1	20816	6.4	9.2	3.8	26.9	7.3	10.6	4.9	32.8
2	20096	4.5	8.4	4.5	36.8	5.8	9.7	5.4	40.6
3	240048	2.9	7.4	4.5	24.4	3.8	8.5	5.4	29
4	320064	7.4	5.6	4.1	21.9	8.4	6.3	5	26.1
5	400080	3.4	5.2	4.1	21	4.1	6.3	5.1	25
6	480096	7	5.1	4.2	28.5	8.3	6.2	5.1	32.4
7	560112	5.2	8.1	3.7	19.9	6.4	9.5	4.9	25.6
8	640128	6.1	4.8	4.3	18.7	7.4	6	5.2	22.3
9	720144	3.9	6.7	3.8	30.5	5.1	8	4.8	34.9
10	800160	7.2	3.1	4.4	21.5	8.7	3.9	5.3	25.5
15	880176	8.5	8.9	3.7	34.1	9.7	10.1	4.9	38.3
20	960192	6.6	5.1	4.7	20.8	8.2	6.1	5.9	26.6
25	2400480	10.5	10.6	5.5	29.1	12.4	14.1	7.8	34.3
Presentation Method 5 (Train on half of replications nearest to the average)									
1	20816	6.4	9.2	3.8	26.9	7.3	10.6	4.9	32.8
2	20096	4.5	8.4	4.5	36.8	5.8	9.7	5.4	40.6
3	9760	5.7	8.1	4.5	24.5	6.9	9.6	5.4	31.1
4	160032	4.7	11.5	4	27.1	5.8	11.9	5	31.4
5	8960	10.7	10.3	4.9	31.8	12.1	11.5	5.8	35.7
6	18432	8.5	6.6	4.7	23.8	9.9	8	5.5	30.4
7	11472	5.4	8.2	4.2	26.8	6.1	9.1	5	33.1
8	31680	8	8.9	3.9	26.6	9.8	10.3	4.8	30.9
9	42304	6.4	8.5	3.8	29.2	7.9	9.7	4.8	33.5
10	26400	10.4	8.3	3.5	29.5	12.1	9.5	4.3	35
15	53440	8.3	8.5	3.6	31.9	10.1	9.6	4.4	36.1
20	480096	4.5	6.5	3.4	20.1	5.4	8	4.2	26.3
25	1200240	4.3	5.3	4	23.2	5.3	6.1	5.5	28.3

Table A9 ANN Results for Experiment 2 on the Test Set

# of Simulation Replications	Mean Cost		Standard Deviation		Minimum Cost		Maximum Cost	
	mae	rmse	mae	rmse	mae	rmse	mae	rmse
Presentation Method 1 (Train on Averages)								
1	10.1	11.5	4.4	35.1	14.9	12.9	7.9	50.7
2	11.1	15.4	6.7	45.2	18.3	19.1	10.6	58.4
3	15.9	15.5	6.2	46.2	21.4	19.4	9.9	57.9
4	10.9	16.8	7	43.7	17.8	20	10.5	55.4
5	12.8	17.6	6.6	46.2	18	21	10.1	59.2
6	9.6	15.3	7	46.9	15.5	19.2	10.3	59.4
7	13.5	17.4	6.8	47.5	18.5	20.8	10	60.6
8	8.4	15.5	7.1	47.7	15.4	19.8	10	60.3
9	12	17	6.9	47	17.4	20.7	10.1	60.2
10	14	16	6.8	47.6	17.3	19.7	9.7	60.5
15	14.4	14.4	6.7	47.9	17.8	18.9	9.5	60.9
20	12.2	16.9	6.8	46.9	17.6	20.1	9.7	60.3
25	11.5	17.2	6.6	47.3	16.8	20.5	9.5	60.2
Presentation Method 2 (Train on averages and individual replications)								
1	10.1	11.5	4.4	35.1	14.9	12.9	7.9	50.7
2	9.7	11	3.8	44	18	14.3	6.2	53.1
3	9.1	8.2	3.7	26.8	15.9	10.5	6	39.2
4	8.3	5.7	4.3	30.4	14.2	8.8	6.7	36.1
5	8.1	8.9	2.6	24.7	12	12	4.2	29
6	11.1	9.2	3.6	22.6	13.2	9.9	6.5	33.5
7	7.2	5.7	2.8	17.8	12.4	7.6	5.6	24.4
8	10.5	6.8	4	28.8	13.7	9.3	7.1	35.2
9	9	10.6	4.7	44.8	13.7	15.3	7.4	49.9
10	10.8	5.5	3.4	28.1	16.3	7.8	4.9	32.6
15	12.4	6.9	2.9	26.6	18.9	8.1	4.1	32.7
20	11.8	10.6	4	30.3	16.4	11.1	5.2	35
25	15.3	15.1	7.5	49.2	26.9	27.6	8.9	106
Presentation Method 3 (Train on averages and half of replications nearest to average)								
1	10.1	11.5	4.4	35.1	14.9	12.9	7.9	50.7
2	8.3	11.2	3.8	40.6	13.9	15	6.4	51.7
3	8.7	9.7	4.4	52	15.6	13.7	6.3	59.6
4	12.6	10.7	3.6	35.5	18	11.4	5.7	40.7
5	7.8	11.9	4.1	38.6	12.3	14	6.3	42.5
6	9.8	11.1	4.5	36.7	15.2	14	6.8	48.1
7	8.3	10.5	3.8	39.7	10.8	13.9	6.8	44
8	11.8	11.7	3.1	30.4	13.9	14.1	4.2	34.5
9	11.8	11.9	3.4	25.4	14.4	15.2	4.2	36.2
10	7.8	7.7	4	38.4	9.7	10	5.7	45.7
15	12.4	8.8	3	27.6	14.7	11.7	3.7	34.3
20	12.1	7.3	4.4	25.7	14.7	8.3	6.3	40.7
25	11.5	8.6	4.6	24.1	23.5	10.7	6.3	37.3

Table A9(Continued) ANN Results for Experiment 2 on the Test Set

# of Simulation Replications	Mean Cost		Standard Deviation		Minimum Cost		Maximum Cost	
	mae	rmse	mae	rmse	mae	rmse	mae	rmse
Presentation Method 4 (Train on all individual replications)								
1	10.1	11.5	4.4	35.1	14.9	12.9	7.9	50.7
2	8.3	11.2	3.8	40.6	13.9	15	6.4	51.7
3	5.7	10.3	3	33.1	13.2	11.6	4.4	40.4
4	11.6	8.9	3.8	26.4	17.2	11.9	6.1	31
5	6.2	7.7	2.7	22	11.9	10.4	4.3	27.2
6	11.7	9.1	3.7	31.9	19.2	11.2	6.6	34.3
7	9.2	10.6	2.9	32.1	13.8	14.3	4.1	50.8
8	11.1	7.2	3.8	23.2	17.8	9.4	7	29.9
9	7.4	8.8	4.1	36.9	14.6	10.2	6.6	41
10	10.2	9.3	3.2	26.6	17.2	15.8	4	32.1
15	11.4	12.5	2.4	43.3	16.3	15.4	3.2	49.7
20	7.9	10.4	3.8	35.2	11.8	19.3	4.7	58.6
25	14.5	13.1	7.4	36.9	18.1	20.3	12.1	42
Presentation Method 5 (Train on the half of replications that are nearest to average)								
1	10.1	11.5	4.4	35.1	14.9	12.9	7.9	50.7
2	8.3	11.2	3.8	40.6	13.9	15	6.4	51.7
3	9.5	9	4.4	32	12	12.3	6	40.2
4	7.6	11.5	3.7	30.4	12.8	12.7	5.3	35.6
5	14.2	12.9	4	38.5	19.1	14.9	6.2	43.2
6	11.2	9.3	4	30.7	16.3	13.5	6.3	39.6
7	8.6	11.4	3.9	37.9	14.3	14.9	6.7	47.3
8	10	12.6	3.8	27.4	12.4	14.9	5.1	31.7
9	8	11.7	3.8	36.3	10.5	15.1	5.1	41.1
10	12.1	12.1	3.4	42	15.4	14.1	4.7	44.8
15	11	11.7	3.6	35.4	18.7	14.2	4.7	41
20	7.6	8	4.1	21.6	13.1	11.8	5.3	27.3
25	21.5	9.7	3.8	53.2	36.3	12.6	5.4	75.8

APPENDIX B

APPENDIX B

DEVELOPMENT PROBLEM 4 PARAMETER INVENTORY SIMULATION COMPUTER PROGRAMS AND RESULTS

```
BEGIN;
PROJECT,       inv4par;
;  The number of distinct training data points is 2500.
;  Total number of replications is  REP x 2500= 25000.
;
VARIABLES: GET:          !Determine which input point to read.
           REP,10:       !REP = # reps to run each data point.
           SmallS:       !s = reorder point.
           SmallD:       !d = order quantity, if I = s.
           I,60:         !Inventory level.
           Io:           !Initial inventory level.
           tba,.1:       !Parameter for time between arrivals.
           k,32:         !Fixed portion of monthly order cost.
           u,5:          !Underage cost.
           w:            !Underage factor.
           Z:            !Amount to order this month.
           BigS:         !S = order up-to quantity.
           AvgInvPlus:   !Equals I, if I>0, else it = 0.
           AvgInvMinus:  !Equals -I, if I<0, else it = 0.
           OrderCost:    !Monthly order cost.
           COST:         !Cumulative order cost.
           TotalCost;    !Avg annual total cost.
;
TALLIES:
       1, Order Costs; !Tallies order cost each month.
;
DSTATS:1,I,INVENTORY:  !Keeps track of inventory levels.
       2,1*AvgInvPlus, !Calculates/tracks cost of overage.
       Excess Inv Cost:!
       3,u*AvgInvMinus,!Calculates/tracks cost of shortages.
       Short Inv Cost; !
;
FILES:
 1,INPUT1,"inv4par.IN", DIR(17)     !File to set
 "(F3.0,1X,F3.0,1X,F3.0,1X,F5.1)": !  input parameters.
 2, OUTPUT1,"inv4par",              !File to receive Write
    SEQ,FREE;                       !  statements.
;
REPLICATE, 25000,0,120;             !Number of replications.
END;
```

Figure B1 Siman Experiment Frame for 4 Input Parameter Inventory Simulation

```
 BEGIN, No,inv4par;
;This is the model frame for the 4 input parameter inventory problem.
;The inputs to the simulation are s (reorder point), d ;(reorder qty),
;k (order costs) and w (factor representing ;u, underage cost).
;The simulation output is average monthly cost, C.
;This uses 3 different Random Number Streams.
;This section obtains the input data at the beginning of each
;replication.  This assumes that each data point is run for Rep # of
;replications.
;
CREATE,    1,0:,1;                        !Do once for each rep.
ASSIGN:    GET=1+AINT((NREP-1)/REP);      !Determines which input data to use.
;                                         !Every REP replications get next
;                                         !  data point.
READ,      INPUT1,                        !Gets data from file
  "(F3.0,1X,F3.0,1X,F3.0,1X,F5.1)",       !  labeled, INPUT1.
  GET:SmallS,SmallD,k,w;                 !SmallS=s=reorder point
;                                         !SmallD=d=order quantity
ASSIGN:    BigS=SmallS + SmallD:          !BigS=order to quantity.
           u=k/w;
DELAY:     0:
           DISPOSE;
;
;
CREATE,   ,EXPONENTIAL(tba,1):            !Arrivals of demands.
           EXPONENTIAL(tba,1);            !Random Stream#1 = 1
BRANCH,    1,4:                           !Levels of demand.
;                                         !Random Stream#2 = 4
           WITH,.167,d1:                  !Demand is 1.
           WITH,.333,d2:                  !Demand is 2.
           WITH,.333,d3:                  !Demand is 3.
           WITH,.167,d4;                  !Demand is 4.
d1 ASSIGN:I = I - 1:                      !Demand set to 1.
           NEXT(d5);
d2 ASSIGN:I = I - 2:                      !Demand set to 2.
           NEXT(d5);
d3 ASSIGN:I = I - 3:                      !Demand set to 3.
           NEXT(d5);
d4 ASSIGN:I = I - 4:                      !Demand set to 4.
           NEXT(d5);
d5 ASSIGN:AvgInvPlus=MX(0,I):             !AvgInvPlus=I, if I>0,
;                                            else, AvgInvPlus = 0.
           AvgInvMinus=MX(0,-I):          !AvgInvMinus=-I, if I<0,
;                                            else, AvgInvMinus=0.
           DISPOSE;
;
;
CREATE,    ,1.0:1.0;                      !Calculate cost at end
;                                         !  of each month.
ASSIGN:    OrderCost = 0;
BRANCH,    1:
           IF,I.ge.SmallS,cost1:          !If inventory is large
;                                         !  enough, go to cost1.
           ELSE,cost2;                    !If inventory is not
;                                            large enough, go to
;                                            cost2.
```

Figure B2 Siman Model Frame for 4 Input Parameter Inventory Simulation

```
cost1     ASSIGN:Z = 0;              !Nothing ordered this month.
          TALLY: 1, OrderCost:
          DISPOSE;
;
cost2     ASSIGN:Z = (BigS-I);       !Order Z amount.
          ASSIGN:OrderCost= k+3*Z;   !Cost spent on orders this month.
          ASSIGN:COST =              !Cumulative cost
                 COST + OrderCost;   !  of orders to date.
          TALLY: 1, OrderCost;
          DELAY: UNIFORM(.5,1.0,8); !Wait for order arrival.
;                                    !Random Stream#3 = 8


ASSIGN:   I = I + Z:                 !Increase inventory by Z
          AvgInvPlus=MX(0,I):        !AvgInvPlus=I, if I>0, ;
;                                    !  else AvgInvPlus = 0.
          AvgInvMinus=MX(0,-I):      !AvgInvMinus=-I, if I<0,
;                                    !  else AvgInvMinus = 0.
          DISPOSE;
;
;
CREATE,   ,120:1,1;                  !After 10 year period,
ASSIGN:   TotalCost=                 !  calculate average
          TAVG(1)+DAVG(2)+DAVG(3);   !  monthly total cost as
;                                    !  the sum of average ;
;                                    !  order,overage &
;                                    !  underage costs.

WRITE,    OUTPUT1,
          "(1X,4(F5.1,1X),F10.5)":
          SmallS, SmallD, k, w, TotalCost:
          DISPOSE;
END;
```

Figure B2 (Continued) Siman Model Frame for 4 Input Parameter Inventory Simulation

TABLE B1 How Training and Testing Data was Generated from SIMAN

Data Type	Number of Points	Number of Replications	Random Number Streams Used
Training	2500	10	1, 4, 8
Testing	900	20	1, 4, 8
Testing	900	20	7, 3, 1
Testing	900	20	2, 6, 10
Testing	900	20	3, 7, 2
Testing	900	20	4, 8, 3
Testing	900	10	5, 9, 4

TABLE B2 Siman Input and Output Data used for Training ANN for the 4 Input Parameter Inventory Simulation (1st 90 Points Run Through SIMAN Simulation)

Point	s	d	k	w	$\overline{C}$	Var($\overline{C}$)	Point	s	d	k	w	$\overline{C}$	Var($\overline{C}$)
1	20	20	16	4	109.11	0.53	46	20	27	80	4	198.59	6.53
2	20	20	16	8	102.03	1.28	47	20	27	80	8	168.14	3.26
3	20	20	16	10.5	101.64	0.68	48	20	27	80	10.5	159.46	3.47
4	20	20	16	13	100.57	0.45	49	20	27	80	13	155.27	3.96
5	20	20	16	17	98.33	0.82	50	20	27	80	17	150.90	1.64
6	20	20	32	4	135.67	5.72	51	20	33	16	4	110.01	0.93
7	20	20	32	8	120.06	1.46	52	20	33	16	8	102.63	0.73
8	20	20	32	10.5	117.85	0.69	53	20	33	16	10.5	101.41	0.42
9	20	20	32	13	116.29	1.65	54	20	33	16	13	99.44	0.62
10	20	20	32	17	114.83	0.32	55	20	33	16	17	100.16	0.15
11	20	20	48	4	161.18	2.38	56	20	33	32	4	129.14	2.44
12	20	20	48	8	143.88	0.97	57	20	33	32	8	118.17	0.94
13	20	20	48	10.5	137.42	2.34	58	20	33	32	10.5	115.48	0.86
14	20	20	48	13	134.19	0.99	59	20	33	32	13	113.71	0.89
15	20	20	48	17	130.56	1.51	60	20	33	32	17	109.99	1.06
16	20	20	64	4	190.49	4.53	61	20	33	48	4	153.27	7.62
17	20	20	64	8	161.76	4.90	62	20	33	48	8	133.04	2.89
18	20	20	64	10.5	155.04	2.12	63	20	33	48	10.5	127.58	1.10
19	20	20	64	13	146.80	1.42	64	20	33	48	13	127.80	1.89
20	20	20	64	17	145.33	1.23	65	20	33	48	17	122.74	1.06
21	20	20	80	4	217.05	11.28	66	20	33	64	4	165.32	9.36
22	20	20	80	8	182.50	1.45	67	20	33	64	8	144.82	1.43
23	20	20	80	10.5	171.12	2.78	68	20	33	64	10.5	141.84	1.07
24	20	20	80	13	165.43	4.43	69	20	33	64	13	133.50	1.05
25	20	20	80	17	161.96	2.01	70	20	33	64	17	134.07	1.61
26	20	27	16	4	108.78	1.16	71	20	33	80	4	192.03	11.37
27	20	27	16	8	102.10	0.33	72	20	33	80	8	161.04	3.23
28	20	27	16	10.5	102.11	0.42	73	20	33	80	10.5	157.69	6.07
29	20	27	16	13	99.62	0.38	74	20	33	80	13	152.09	1.56
30	20	27	16	17	98.81	0.51	75	20	33	80	17	144.29	2.62
31	20	27	32	4	133.15	1.72	76	20	40	16	4	109.74	0.85
32	20	27	32	8	117.85	3.10	77	20	40	16	8	104.76	0.63
33	20	27	32	10.5	115.72	1.78	78	20	40	16	10.5	102.35	0.37
34	20	27	32	13	113.75	1.17	79	20	40	16	13	102.74	0.22
35	20	27	32	17	113.07	0.49	80	20	40	16	17	101.57	0.60
36	20	27	48	4	152.83	3.66	81	20	40	32	4	126.23	1.28
37	20	27	48	8	135.97	2.58	82	20	40	32	8	117.04	1.74
38	20	27	48	10.5	128.62	1.81	83	20	40	32	10.5	114.53	0.74
39	20	27	48	13	128.15	1.05	84	20	40	32	13	114.29	1.42
40	20	27	48	17	123.90	1.62	85	20	40	32	17	111.26	0.41
41	20	27	64	4	180.18	13.14	86	20	40	48	4	146.06	5.82
42	20	27	64	8	152.35	2.21	87	20	40	48	8	128.27	1.95
43	20	27	64	10.5	145.36	2.28	88	20	40	48	10.5	127.51	0.60
44	20	27	64	13	141.12	1.21	89	20	40	48	13	123.36	2.00
45	20	27	64	17	137.42	1.46	90	20	40	48	17	120.96	1.18

Table B3 Simulation Data for Training Set F (144 points shuffled)

s	d	k	w	$\overline{C}$	Var($\overline{C}$)		s	d	k	w	$\overline{C}$	Var($\overline{C}$)
40	80	48	10.5	144.08	0.41		20	80	80	4	161.12	6.49
80	80	16	4	176.02	0.40		60	80	16	17	155.16	0.37
40	60	48	10.5	136.44	0.71		20	60	80	4	172.44	9.88
80	60	16	4	166.40	0.24		60	60	16	17	145.63	0.11
40	40	48	10.5	133.92	0.83		20	40	80	4	179.56	16.53
80	40	16	4	156.80	0.19		60	40	16	17	137.30	0.39
40	20	48	10.5	139.95	0.58		20	20	80	4	217.05	11.28
80	20	16	4	153.05	0.42		60	20	16	17	132.21	0.33
20	80	48	10.5	131.21	0.76		80	80	80	10.	192.66	0.60
60	80	16	4	154.45	0.42		40	80	16	17	136.11	0.63
20	60	48	10.5	126.76	2.18		80	60	80	10.	188.22	0.51
60	60	16	4	147.46	0.46		40	60	16	17	125.53	0.46
20	40	48	10.5	127.50	0.60		80	40	80	10.	185.55	0.76
60	40	16	4	136.83	0.55		40	40	16	17	116.01	0.33
20	20	48	10.5	137.42	2.34		80	20	80	10.	202.70	1.15
60	20	16	4	133.11	0.42		40	20	16	17	113.36	0.46
80	80	48	17	183.85	0.30		60	80	80	10.	173.13	0.74
40	80	16	4	134.56	0.34		20	80	16	17	118.08	0.21
80	60	48	17	176.49	0.47		60	60	80	10.	168.47	1.15
40	60	16	4	126.80	0.38		20	60	16	17	109.16	0.29
80	40	48	17	173.10	0.24		60	40	80	10.	166.21	1.42
40	40	16	4	117.71	0.59		20	40	16	17	101.57	0.60
80	20	48	17	176.64	0.58		60	20	80	10.	182.84	1.12
40	20	16	4	113.93	0.64		20	20	16	17	98.33	0.82
60	80	48	17	163.39	0.59		40	80	80	10.	152.67	0.77
20	80	16	4	121.53	0.77		80	80	48	4	184.56	1.13
60	60	48	17	155.38	0.43		40	60	80	10.	147.95	0.87
20	60	16	4	114.45	0.82		80	60	48	4	177.84	0.61
60	40	48	17	151.72	0.22		40	40	80	10.	147.71	0.51
20	40	16	4	109.74	0.85		80	40	48	4	172.53	0.21
60	20	48	17	155.53	1.20		40	20	80	10.	164.42	1.90
20	20	16	4	109.11	0.53		80	20	48	4	177.01	1.09
40	80	48	17	143.02	0.49		20	80	80	10.	144.85	1.09
80	80	16	10.5	175.65	0.12		60	80	48	4	162.82	0.92
40	60	48	17	138.02	0.50		20	60	80	10.	142.00	0.60
80	60	16	10.5	165.68	0.38		60	60	48	4	158.23	0.44
40	40	48	17	133.02	1.07		20	40	80	10.	148.23	1.25
80	40	16	10.5	157.32	0.37		60	40	48	4	152.67	0.74
40	20	48	17	137.39	0.63		20	20	80	10.	171.12	2.78
80	20	16	10.5	152.07	0.36		60	20	48	4	157.41	0.62
20	80	48	17	129.17	0.34		80	80	80	17	192.38	0.66
60	80	16	10.5	155.44	0.23		40	80	48	4	145.87	0.86
20	60	48	17	123.34	0.77		80	60	80	17	188.43	0.45
60	60	16	10.5	145.88	0.32		40	60	48	4	138.00	0.87

Table B3 (Continued) Simulation Data for Training Set F (144 points)

s	d	k	w	$\overline{C}$	Var($\overline{C}$)		s	d	k	w	$\overline{C}$	Var($\overline{C}$)
20	40	48	17	120.96	1.18		80	40	80	17	187.53	1.28
60	40	16	10.5	136.74	0.44		40	40	48	4	136.70	0.57
20	20	48	17	130.56	1.51		80	20	80	17	200.96	2.68
60	20	16	10.5	131.56	0.52		40	20	48	4	140.05	1.09
80	80	80	4	192.63	0.62		60	80	80	17	172.85	0.83
40	80	16	10.5	134.57	0.42		20	80	48	4	140.69	2.13
80	60	80	4	187.24	0.59		60	60	80	17	168.32	0.56
40	60	16	10.5	126.04	0.38		20	60	48	4	144.18	4.82
80	40	80	4	187.47	0.63		60	40	80	17	166.24	1.51
40	40	16	10.5	118.93	0.34		20	40	48	4	146.06	5.82
80	20	80	4	202.05	2.94		60	20	80	17	181.98	1.15
40	20	16	10.5	114.34	0.34		20	20	48	4	161.18	2.38
60	80	80	4	172.22	0.75		40	80	80	17	154.21	0.21
20	80	16	10.5	118.02	0.36		80	80	48	10.5	183.80	0.30
60	60	80	4	167.13	0.73		40	60	80	17	148.96	1.16
20	60	16	10.5	109.12	0.64		80	60	48	10.5	177.27	0.58
60	40	80	4	168.60	0.98		40	40	80	17	147.47	0.43
20	40	16	10.5	102.35	0.37		80	40	48	10.5	172.70	0.39
60	20	80	4	181.70	1.01		40	20	80	17	162.34	1.04
20	20	16	10.5	101.64	0.68		80	20	48	10.5	177.85	0.65
40	80	80	4	155.61	1.00		20	80	80	17	140.28	0.95
80	80	16	17	175.90	0.74		60	80	48	10.5	163.70	0.39
40	60	80	4	149.74	0.30		20	60	80	17	137.48	0.61
80	60	16	17	166.38	0.07		60	60	48	10.5	155.76	0.23
40	40	80	4	152.82	1.37		20	40	80	17	140.61	2.48
80	40	16	17	158.96	0.21		60	40	48	10.5	152.71	0.05
40	20	80	4	170.76	3.68		20	20	80	17	161.96	2.01
80	20	16	17	152.54	0.58		60	20	48	10.5	158.35	0.48

Table B4 Test Set with 0 Parameter Values External to the Training Sets

s	d	k	w	$\overline{C}$	Var($\overline{C}$)	s	d	k	w	$\overline{C}$	Var($\overline{C}$)
30	30	24	6	113.50	0.87	50	50	56	6	148.00	0.70
30	30	24	9	112.50	0.62	50	50	56	9	147.42	0.59
30	30	24	12	111.37	0.76	50	50	56	12	147.63	0.54
30	30	24	15	110.74	0.67	50	50	56	15	147.19	0.51
30	30	40	6	126.11	1.33	50	50	72	6	154.03	0.81
30	30	40	9	123.00	1.00	50	50	72	9	153.90	0.58
30	30	40	12	122.30	0.98	50	50	72	12	154.19	0.68
30	30	40	15	121.31	0.66	50	50	72	15	153.79	0.67
30	30	56	6	138.80	2.66	50	70	24	6	143.30	0.47
30	30	56	9	134.41	1.09	50	70	24	9	142.75	0.36
30	30	56	12	132.42	0.85	50	70	24	12	142.79	0.49
30	30	56	15	130.72	0.80	50	70	24	15	142.62	0.56
30	30	72	6	151.32	3.19	50	70	40	6	148.20	0.51
30	30	72	9	145.57	1.59	50	70	40	9	147.63	0.55
30	30	72	12	142.90	1.37	50	70	40	12	147.72	0.36
30	30	72	15	141.10	1.31	50	70	40	15	147.40	0.57
30	50	24	6	118.41	0.69	50	70	56	6	153.11	0.67
30	50	24	9	117.12	0.52	50	70	56	9	152.52	0.47
30	50	24	12	116.37	0.62	50	70	56	12	153.04	0.58
30	50	24	15	115.83	0.63	50	70	56	15	152.43	0.72
30	50	40	6	126.13	0.85	50	70	72	6	157.51	0.68
30	50	40	9	123.98	0.71	50	70	72	9	157.30	0.64
30	50	40	12	123.63	0.61	50	70	72	12	157.07	0.59
30	50	40	15	123.57	0.66	50	70	72	15	157.44	0.61
30	50	56	6	135.19	1.09	70	30	24	6	147.89	0.46
30	50	56	9	132.43	0.95	70	30	24	9	148.33	0.38
30	50	56	12	131.32	0.85	70	30	24	12	147.83	0.46
30	50	56	15	130.37	0.69	70	30	24	15	148.35	0.49
30	50	72	6	143.63	1.20	70	30	40	6	156.52	0.39
30	50	72	9	140.38	1.27	70	30	40	9	156.99	0.67
30	50	72	12	138.56	1.13	70	30	40	12	157.32	0.60
30	50	72	15	137.59	0.67	70	30	40	15	157.32	0.56
30	70	24	6	125.26	0.67	70	30	56	6	166.14	0.50
30	70	24	9	125.08	0.56	70	30	56	9	166.21	0.71
30	70	24	12	123.84	0.34	70	30	56	12	165.81	0.67
30	70	24	15	123.88	0.44	70	30	56	15	165.91	0.62
30	70	40	6	132.06	0.83	70	30	72	6	174.31	0.63
30	70	40	9	130.43	0.63	70	30	72	9	174.66	0.72
30	70	40	12	129.33	0.61	70	30	72	12	175.16	0.83
30	70	40	15	129.48	0.55	70	30	72	15	174.96	0.86
30	70	56	6	138.39	1.05	70	50	24	6	154.75	0.43
30	70	56	9	136.17	0.71	70	50	24	9	155.19	0.36
30	70	56	12	135.02	0.69	70	50	24	12	154.99	0.46
30	70	56	15	134.96	0.76	70	50	24	15	155.11	0.55

Table B4(Continued) Test Set with 0 Parameter Values External to the Training Sets

s	d	k	w	$\overline{C}$	Var($\overline{C}$)	s	d	k	w	$\overline{C}$	Var($\overline{C}$)
30	70	72	6	145.22	1.74	70	50	40	6	161.21	0.53
30	70	72	9	142.06	0.82	70	50	40	9	161.17	0.64
30	70	72	12	140.56	1.06	70	50	40	12	161.51	0.54
30	70	72	15	140.15	0.91	70	50	40	15	161.12	0.50
50	30	24	6	128.28	0.41	70	50	56	6	168.06	0.54
50	30	24	9	127.89	0.47	70	50	56	9	167.30	0.62
50	30	24	12	128.54	0.45	70	50	56	12	167.18	0.72
50	30	24	15	127.86	0.38	70	50	56	15	167.89	0.79
50	30	40	6	137.80	0.62	70	50	72	6	173.69	0.75
50	30	40	9	136.63	0.47	70	50	72	9	173.57	0.69
50	30	40	12	136.81	0.43	70	50	72	12	173.20	0.73
50	30	40	15	137.31	0.68	70	50	72	15	174.22	0.63
50	30	56	6	146.35	0.91	70	70	24	6	163.34	0.44
50	30	56	9	145.69	1.13	70	70	24	9	162.73	0.55
50	30	56	12	146.29	0.64	70	70	24	12	162.89	0.55
50	30	56	15	146.34	0.79	70	70	24	15	162.85	0.38
50	30	72	6	155.40	0.87	70	70	40	6	167.60	0.53
50	30	72	9	155.90	0.92	70	70	40	9	167.81	0.57
50	30	72	12	155.09	0.85	70	70	40	12	167.90	0.55
50	30	72	15	155.28	1.00	70	70	40	15	168.01	0.57
50	50	24	6	134.80	0.46	70	70	56	6	172.76	0.52
50	50	24	9	135.03	0.59	70	70	56	9	172.64	0.66
50	50	24	12	134.66	0.39	70	70	56	12	172.83	0.60
50	50	24	15	134.76	0.36	70	70	56	15	172.70	0.79
50	50	40	6	141.58	0.43	70	70	72	6	177.34	0.60
50	50	40	9	141.18	0.55	70	70	72	9	177.58	0.57
50	50	40	12	141.39	0.66	70	70	72	12	177.59	0.55
50	50	40	15	141.40	0.51	70	70	72	15	177.26	0.76

```
n1f5.det
input number 1 4
output number 1 1
hidden 5 5
filename trainfacts m1b.fct
filename testfacts m1d.tst
filename teststats n1f5.sta
filename trainstats n1f5 sts
learnrate  1.0000 50  1.0000 75  1.0000 90  1.0000
learnlayer  1.0000  1.0000  1.0000
traintol  0.0200  0.0200  0.8000 100
testtol  0.0200
maxruns 750
smoothing  0.9000  0.9000  0.9000
testruns 1
function hidden1 sigmoid  0.0000  1.0000  0.0000 1.0000
function hidden2 sigmoid  0.0000  1.0000  0.0000 1.0000
function output sigmoid  0.0000  1.0000  0.0000 1.0000
dictionary input s d k w
dictionary output tc
scale input minimum
2.0000 2.0000 0.000 1.5000
scale input maximum
98.000 98.000 96.000 19.500
scale output minimum
45.680
scale output maximum
554.17
statistics 0 0 0
weights 4 1 4 5 5 1
-2.3886  1.0226 -0.0402 -1.6250 -2.1146
 0.8540  1.3142  1.7564  2.0830 -3.4422
-3.4214 -1.1646 -2.8056  0.3094  1.3136
 4.6552 -3.9432 -1.2824  3.2806  4.2112
 1.5944 -2.4754  2.6724  1.6484  0.0960

 1.3756 -3.2220 -1.9236  1.3374  0.9496 -1.3140
 1.6766  1.1110 -0.9690 -0.4576 -0.8770 -1.4986
-4.7440  0.0316  0.8292  1.9126 -3.4686 -2.0884
 2.0272  0.4896  0.7032  0.2432  5.2260 -1.1908
 2.6908 -1.0842  1.8292  0.5574  0.5990 -2.8316

 0.7232 -1.6782 -2.2422  1.4250 -0.3066  2.1650
```

Figure B3 Initial BrainMaker Training File for Predicting Mean Cost

```
n1f5.net
input number 1 4
output number 1 1
hidden 5 5
filename trainfacts m1b.fct
filename testfacts m1d.tst
filename teststats n5.sta
filename trainstats n5.sts
learnrate  1.0000 50  1.0000 75  1.0000 90  1.0000
learnlayer  1.0000  1.0000  1.0000
traintol  0.0200  0.0200  0.8000 100
testtol  0.0200
maxruns 58
smoothing  0.9000  0.9000  0.9000
testruns 58
function hidden1 sigmoid  0.0000  1.0000  0.0000 1.0000
function hidden2 sigmoid  0.0000  1.0000  0.0000 1.0000
function output sigmoid  0.0000  1.0000  0.0000 1.0000
dictionary input s d k w
dictionary output tc
outputfile n1f5.out number none  number number none  0 0 0
scale input minimum
2.0000 2.0000 0.000 1.5000
scale input maximum
98.000 98.000 96.000 19.500
scale output minimum
45.680
scale output maximum
554.17
statistics 83520 11670 58
weights 4 1 4 5 5 1
-1.6830 -3.2044  1.3186 -0.1604 -0.8976
-7.9998 -5.1952 -4.6116 -5.1224 -5.5262
-3.3516 -1.9562 -0.4174 -0.1970  1.9582
 7.2766  0.5708 -2.2656  3.9482  0.8004
 7.9994  6.5356  7.9994  4.3016  7.9994

 1.4716 -7.9998 -4.6276 -0.4610  0.4430 -1.8644
 7.3596 -4.3536  1.9686 -7.9998 -7.9998 -7.9998
-4.9430  0.0456  2.2070  3.2404 -2.6000 -0.9274
 2.0272 -7.9998 -3.1106 -7.9998 -7.7506 -7.9998
 2.6908 -0.8932  4.8906 -7.9998 -7.9998 -7.9998
 5.6852  0.9166 -2.9240  4.2820  1.7166 -0.2710
```

Figure B4 Trained BrainMaker File for Predicting Mean Cost Using Replications

```
p1f5.net
input number 1 4
output number 1 1
hidden 5 5
filename trainfacts m1b.fct
filename testfacts m1d.tst
filename teststats p5.sta
filename trainstats p5.sts
learnrate  1.0000 50  1.0000 75  1.0000 90  1.0000
learnlayer  1.0000  1.0000  1.0000
traintol  0.0200  0.0200  0.8000 100
testtol  0.0200
maxruns 152
smoothing  0.9000  0.9000  0.9000
testruns 152
function hidden1 sigmoid  0.0000  1.0000  0.0000 1.0000
function hidden2 sigmoid  0.0000  1.0000  0.0000 1.0000
function output sigmoid  0.0000  1.0000  0.0000 1.0000
dictionary input s d k w
dictionary output tc
outputfile p1f5.out number none  number number none  0 0 0
scale input minimum
2.0000 2.0000 0.000 1.5000
scale input maximum
98.000 98.000 96.000 19.500
scale output minimum
45.680
scale output maximum
554.17

statistics 21888 7266 152
weights 4 1 4 5 5 1
-7.9998 -4.9002  2.4908 -7.5008  1.1516
-6.0876 -5.6052 -5.1972  0.4470 -7.9998
-5.1606 -0.5892 -2.8364 -0.0016  3.6640
 7.9994  2.2654 -3.2764  7.9994  2.8010
 7.9994  4.1814  7.9994  3.1772  7.9994

 1.3756 -7.9998 -6.8974 -0.2350 -0.5386 -2.8802
 5.2116 -2.1682  0.9246 -7.9998 -7.9998 -7.9998
-2.7630  0.0772  1.4322  2.9976 -2.5900 -0.9472
 0.2592 -5.2496 -5.0276 -7.9998 -3.4742 -7.9998
 2.6908 -0.9572  3.8272 -7.3514 -7.3996 -7.9998

 3.5646 -0.1260 -2.9326  0.7674 -0.9014  0.0832
```

Figure B5 Trained BrainMaker File for Predicting Mean Cost Using Averages

```
v1f5.det
input number 1 4
output number 1 1
hidden 5 5
filename trainfacts v1f.fct
filename testfacts v1.tst
filename trainstats v1f5.sts
filename teststats v1f5.sta
learnrate  1.0000 50  1.0000 75  1.0000 90  1.0000
learnlayer  1.0000  1.0000  1.0000
traintol  0.0020  0.0020  0.8000 100
testtol  0.0020
maxruns 750
smoothing  0.9000  0.9000  0.9000
testruns 1
function hidden1 sigmoid  0.0000  1.0000  0.0000 1.0000
function hidden2 sigmoid  0.0000  1.0000  0.0000 1.0000
function output sigmoid  0.0000  1.0000  0.0000 1.0000
dictionary input s d k w
dictionary output var
scale input minimum
2.0000 2.0000 0.000 1.5000
scale input maximum
98.000 98.000 96.000 19.500
scale output minimum
-4.851
scale output maximum
53.816
statistics 0 0 0
weights 4 1 4 5 5 1
-2.3886  1.0226 -0.0402 -1.6250 -2.1146
 0.8540  1.3142  1.7564  2.0830 -3.4422
-3.4214 -1.1646 -2.8056  0.3094  1.3136
 4.6552 -3.9432 -1.2824  3.2806  4.2112
 1.5944 -2.4754  2.6724  1.6484  0.0960

 1.3756 -3.2220 -1.9236  1.3374  0.9496 -1.3140
 1.6766  1.1110 -0.9690 -0.4576 -0.8770 -1.4986
-4.7440  0.0316  0.8292  1.9126 -3.4686 -2.0884
 2.0272  0.4896  0.7032  0.2432  5.2260 -1.1908
 2.6908 -1.0842  1.8292  0.5574  0.5990 -2.8316

 0.7232 -1.6782 -2.2422  1.4250 -0.3066  2.1650
```

Figure B6 Initial BrainMaker File for Predicting Variance ($\overline{C}$)

```
v1f5.net
input number 1 4
output number 1 1
hidden 5 5
filename trainfacts v1f.fct
filename testfacts v1.tst
filename trainstats v5.sts
filename teststats v5.sta
learnrate 1.0000 50 1.0000 75 1.0000 90 1.0000
learnlayer 1.0000 1.0000 1.0000
traintol 0.0020 0.0020 0.8000 100
testtol 0.0020
maxruns 545
smoothing 0.9000 0.9000 0.9000
testruns 545
function hidden1 sigmoid 0.0000 1.0000 0.0000 1.0000
function hidden2 sigmoid 0.0000 1.0000 0.0000 1.0000
function output sigmoid 0.0000 1.0000 0.0000 1.0000
dictionary input s d k w
dictionary output var
outputfile v1f5.out number none number number none 0 0 0
scale input minimum
2.0000 2.0000 0.000 1.5000
scale input maximum
98.000 98.000 96.000 19.500
scale output minimum
-4.851
scale output maximum
53.816
statistics 78480 69595 545
weights 4 1 4 5 5 1
-3.9144 -4.3062 -4.5060 -3.1040 -4.1776
-5.8854 -6.9462 -7.9994 -5.0092 -7.9994
 7.9236  0.9502 -3.8764  7.9242 -1.1420
 7.7452  0.7354 -4.4396  7.7452  0.2684
 3.6664 -3.1624 -7.9994  1.7496 -7.9994

 1.3756 -7.9994 -2.8502  2.2260 -0.9610 -2.8886
 7.9994  1.3040 -2.1364  1.5154 -2.8666 -3.3582
 7.9994  7.9994 -2.2608 -3.1126  3.8222  0.0310
-7.9994 -7.9994 -0.6666 -2.4742  5.8654 -3.8292
 2.6908 -0.8790  4.3396 -2.3684  1.0252 -6.1110

 7.2670  6.7960  5.3484  7.2126  4.5642 -2.6802
```

Figure B7 Trained BrainMaker File for Predicting Variance ($\overline{C}$)

APPENDIX C

APPENDIX C

DEMONSTRATION PROBLEM ED RESULTS

Table C1 ANN Training Data for Emergency Department Simulation

ICBWT	GCBWT	LABT	XRAYT	$\overline{T}$	Var($\overline{T}$)
0	79	36	0	121.63	23.50
0	158	72	50	154.03	22.66
75	79	0	100	160.86	12.79
75	158	72	0	129.91	7.75
150	79	0	50	139.50	9.64
150	158	36	100	165.65	32.43
0	0	72	50	138.56	15.52
0	158	0	100	149.82	36.84
75	0	72	0	124.10	24.76
75	158	0	50	142.91	20.25
150	0	36	100	180.40	106.26
150	158	0	0	118.94	24.55
0	0	0	100	159.04	23.08
0	79	72	0	123.95	26.13
75	0	0	50	133.83	23.08
75	79	36	100	166.09	18.15
150	0	0	0	115.45	9.11
150	79	36	50	140.73	52.38
150	158	72	100	188.03	361.99
0	79	0	50	131.73	17.10
0	158	36	100	174.08	71.18
75	79	0	0	122.94	14.58
75	158	36	50	146.18	24.76
150	0	72	100	177.57	65.93
150	158	36	0	129.26	18.99
0	0	36	100	154.61	19.62
0	158	0	0	117.20	11.32
75	0	36	50	142.55	13.95
75	79	72	100	164.27	22.03
150	0	36	0	119.23	12.89
150	79	72	50	151.27	45.87
0	0	0	0	110.51	11.21
0	79	36	50	144.73	60.47
0	158	72	100	163.40	36.84
75	79	36	0	119.38	7.75
75	158	72	50	153.37	130.94

Table C1(Continued) ANN Training Data for Emergency Department Simulation

ICBWT	GCBWT	LABT	XRAYT	$\bar{\bar{T}}$	Var($\bar{\bar{T}}$)
150	79	0	100	167.83	31.90
150	158	72	0	131.87	45.03
0	0	72	100	157.37	12.79
0	158	36	0	114.94	10.06
75	0	72	50	142.04	19.93
75	158	0	100	172.05	18.36
150	0	72	0	133.25	43.88
150	158	0	50	138.34	17.20
0	0	36	0	115.60	17.83
0	79	72	50	147.56	25.81
75	0	0	100	151.27	23.19
75	79	72	0	130.71	12.37
150	0	0	50	145.09	41.25
150	79	36	100	175.17	52.91
75	79	36	50	153.88	51.23
0	79	0	100	166.38	53.64
0	158	72	0	131.36	8.06
75	79	0	50	137.83	15.00
75	158	36	100	168.85	48.50
150	79	0	0	113.64	6.59
150	158	36	50	143.13	12.47
0	0	72	0	117.71	9.74
0	158	0	50	144.29	11.74
75	0	36	100	158.90	38.94
75	158	0	0	114.15	8.06
150	0	36	50	138.05	9.22
150	79	72	100	175.46	32.01
0	0	0	50	135.87	27.70
0	79	36	100	168.70	31.69
75	0	0	0	112.18	16.05
150	0	72	50	145.53	14.58
75	158	72	100	171.97	25.18
150	79	36	0	124.03	3.44
150	158	72	50	152.94	7.33
0	79	0	0	111.97	9.43
0	158	36	50	139.94	22.35
75	0	72	100	167.18	46.61
75	158	36	0	118.21	4.91
75	0	36	0	114.00	12.26
150	158	0	100	178.73	85.47
0	0	36	50	135.50	20.56
0	79	72	100	164.27	13.84
150	0	0	100	161.73	72.34
75	79	72	50	142.70	20.88
150	79	72	0	128.89	14.58

Table C2 ANN Testing Data for Emergency Department Simulation

ICBWT	GCBWT	LABT	XRAYT	$\overline{T}$	Var($\overline{T}$)
12	12.64	5.76	8	115.3	10.16
12	12.64	5.76	92	152.7	35.47
12	12.64	66.24	8	123.8	16.15
12	12.64	66.24	92	161.8	72.86
12	145.36	5.76	8	119.6	11.84
12	145.36	5.76	92	157	27.28
12	145.36	66.24	8	128.8	17.62
12	145.36	66.24	92	169.5	57.32
138	12.64	5.76	8	119.5	12.26
138	12.64	5.76	92	156.5	24.44
138	12.64	66.24	8	128.2	11.73
138	12.64	66.24	92	165.7	44.4
138	145.36	5.76	8	124.8	12.47
138	145.36	5.76	92	164	46.29
138	145.36	66.24	8	132.8	13.73
138	145.36	66.24	92	180.6	97.96
24.75	26.07	11.88	16.5	118.8	11.63
24.75	26.07	11.88	83.5	150.4	27.8
24.75	26.07	60.12	16.5	126.2	13.73
24.75	26.07	60.12	83.5	154.9	25.49
24.75	131.93	11.88	16.5	124.9	16.46
24.75	131.93	11.88	83.5	158.3	57.11
24.75	131.93	60.12	16.5	129.6	15.83
24.75	131.93	60.12	83.5	162.6	55.84
125.25	26.07	11.88	16.5	123.3	17.62
125.25	26.07	11.88	83.5	155.9	39.04
125.25	26.07	60.12	16.5	129.9	12.15
125.25	26.07	60.12	83.5	163	40.93
125.25	131.93	11.88	16.5	127.4	13.42
125.25	131.93	11.88	83.5	162.5	29.8
125.25	131.93	60.12	16.5	136.3	18.25
125.25	131.93	60.12	83.5	170	45.97
37.5	39.5	18	25	125.5	17.41
37.5	39.5	18	75	152.2	28.33
37.5	39.5	54	25	129.6	17.93
37.5	39.5	54	75	153	38.31
37.5	118.5	18	25	129.3	17.72
37.5	118.5	18	75	150.6	32.21
37.5	118.5	54	25	134.3	20.14
37.5	118.5	54	75	159.3	34.74
112.5	39.5	18	25	129.1	18.04
112.5	39.5	18	75	150.1	29.9
112.5	39.5	54	25	132	14.78
112.5	39.5	54	75	157	33.89
112.5	118.5	18	25	130.7	18.88
112.5	118.5	18	75	155.8	61.73
112.5	118.5	54	25	136.7	26.86
112.5	118.5	54	75	161	44.71

Table C2(Continued) ANN Testing Data for Emergency Department Simulation

ICBWT	GCBWT	LABT	XRAYT	$\overline{T}$	Var($\overline{T}$)
50.25	52.93	24.12	33.5	132.2	11.94
50.25	52.93	24.12	66.5	145	19.93
50.25	52.93	47.88	33.5	136.4	24.65
50.25	52.93	47.88	66.5	151.9	25.91
50.25	105.07	24.12	33.5	135.2	21.5
50.25	105.07	24.12	66.5	148.2	17.72
50.25	105.07	47.88	33.5	136.5	19.51
50.25	105.07	47.88	66.5	154	34.31
99.75	52.93	24.12	33.5	134.8	22.13
99.75	52.93	24.12	66.5	148.2	42.3
99.75	52.93	47.88	33.5	135.8	15.52
99.75	52.93	47.88	66.5	154.5	34.84
99.75	105.07	24.12	33.5	135.2	15.94
99.75	105.07	24.12	66.5	152	39.15
99.75	105.07	47.88	33.5	140.3	25.18
99.75	105.07	47.88	66.5	153.1	20.98
63	66.36	30.24	42	140.2	22.24
63	66.36	30.24	58	148.1	39.15
63	66.36	41.76	42	139.5	25.6
63	66.36	41.76	58	146.2	22.55
63	91.64	30.24	42	140.4	24.23
63	91.64	30.24	58	145.1	23.18
63	91.64	41.76	42	139.4	14.68
63	91.64	41.76	58	147.1	20.87
87	66.36	30.24	42	138.7	23.39
87	66.36	30.24	58	146.4	26.86
87	66.36	41.76	42	141.8	29.8
87	66.36	41.76	58	149.4	27.7
87	91.64	30.24	42	136.6	22.24
87	91.64	30.24	58	144.8	32.32
87	91.64	41.76	42	140	20.87
87	91.64	41.76	58	151.8	30.22

```
input number 1 4
output number 1 1
hidden 4 4

filename trainfacts ee.fct
filename testfacts ed.tst
filename trainstats fee.sts
filename teststats fee.sta
learnrate  1.0000 50  1.0000 75  1.0000 90  1.0000
learnlayer  1.0000  1.0000  1.0000
traintol  0.0020  0.0020  0.8000 100
testtol  0.0020
maxruns 1000
smoothing  0.9000  0.9000  0.9000
testruns 1
function hidden1 sigmoid  0.0000  1.0000  0.0000 1.0000
function hidden2 sigmoid  0.0000  1.0000  0.0000 1.0000
function output sigmoid  0.0000  1.0000  0.0000 1.0000
dictionary input int gen lab xray
dictionary output time

display network progress
scale input minimum
0.0000 0.0000 0.000 0.0000
scale input maximum
150.000 158.000 72.000 100.000
scale output minimum
102.72
scale output maximum
195.76
statistics 0 0 0
weights 4 1 4 4 4 1
-3.8554 -0.4276 -0.3262  0.9382 -0.8782
 3.7434  1.4926 -3.1036  2.8272 -1.2676
-0.3316 -3.0782 -1.7292  0.1736 -0.7512
 2.7450  4.5422 -4.1044 -0.1690 -2.7670

-0.4850  1.8116  0.0434  0.2844 -1.9114
-0.6790 -0.2360 -2.7194  0.7742 -2.0874
-2.1076 -0.5446  0.3944 -2.8502  1.2972
 1.4124  2.2090  0.0920 -2.0208  5.7212

-5.1514  2.1156  1.7940 -3.9106  1.7380
```

Figure C1 Initial Brainmaker File for Predicting Mean Time in the ED($\overline{T}$) Using Averages (PM 1)

```
input number 1 4
output number 1 1
hidden 4 4

filename trainfacts ee.fct
filename testfacts ee.tst
filename trainstats fee.sts
filename teststats fee.sta
learnrate 1.0000 50 1.0000 75 1.0000 90 1.0000
learnlayer 1.0000 1.0000 1.0000
traintol 0.0020 0.0020 0.8000 100
testtol 0.0020
maxruns 870
smoothing 0.9000 0.9000 0.9000
testruns 870
function hidden1 sigmoid 0.0000 1.0000 0.0000 1.0000
function hidden2 sigmoid 0.0000 1.0000 0.0000 1.0000
function output sigmoid 0.0000 1.0000 0.0000 1.0000
dictionary input int gen lab xray
dictionary output time
outputfile feetst.out number none number number none 0 0 0
scale input minimum
0.000 0.000 0.000 0.000
scale input maximum
150.00 158.00 72.000 100.00
scale output minimum
102.72
scale output maximum
195.76
statistics 70470 68283 870
weights 4 1 4 4 4 1
-5.2926 -1.4212 7.8330 -5.3380 1.3412
 7.9994 6.9524 7.9994 6.9524 4.7766
-0.1862 -0.2516 -0.9108 -3.1192 1.6252
 7.9994 7.9994 0.3682 5.4096 -6.5080

-0.2046 -0.5696 3.7282 -0.2874 -2.4508
-0.2704 0.8236 -5.2504 1.0544 -2.6404
-1.6120 1.5260 1.7024 -1.8156 1.0020
 7.9994 6.4254 -1.4096 -3.5294 7.9994

-4.6394 5.6714 0.6206 -2.5634 2.0570
```

Figure C2 Trained Brainmaker File for Predicting Mean Time in the ED($\overline{T}$) Using Averages (PM 1)

```
input number 1 4
output number 1 1
hidden 4 4

filename trainfacts ed.fct
filename testfacts ed.tst
filename trainstats fed.sts
filename teststats fed.sta

learnrate  1.0000 50  1.0000 75  1.0000 90  1.0000
learnlayer  1.0000  1.0000  1.0000
traintol  0.0020  0.0020  0.8000 100
testtol  0.0020
maxruns 1000
smoothing  0.9000  0.9000  0.9000
testruns 1
function hidden1 sigmoid  0.0000  1.0000  0.0000 1.0000
function hidden2 sigmoid  0.0000  1.0000  0.0000 1.0000
function output sigmoid  0.0000  1.0000  0.0000 1.0000
dictionary input int gen lab xray
dictionary output time
display network progress
scale input minimum
0.0000 0.0000 0.000 0.0000
scale input maximum
150.000 158.000 72.000 100.000
scale output minimum
69.01
scale output maximum
366.57
statistics 0 0 0
weights 4 1 4 4 4 1
-3.8554 -0.4276 -0.3262  0.9382 -0.8782
 3.7434  1.4926 -3.1036  2.8272 -1.2676
-0.3316 -3.0782 -1.7292  0.1736 -0.7512
 2.7450  4.5422 -4.1044 -0.1690 -2.7670

-0.4850  1.8116  0.0434  0.2844 -1.9114
-0.6790 -0 .2360 -2.7194  0.7742 -2.0874
-2.1076 -0.5446  0.3944 -2.8502  1.2972
 1.4124  2.2090  0.0920 -2.0208  5.7212

-5.1514  2.1156  1.7940 -3.9106  1.7380
```

Figure C3 Initial Brainmaker File for Predicting Mean Time in the ED($\overline{T}$) Using Individual Replications (PM 4)

```
input number 1 4
output number 1 1
hidden 4 4

filename trainfacts ed.fct
filename testfacts ed.tst
filename trainstats fed.sts
filename teststats fed.sta
learnrate 1.0000 50 1.0000 75 1.0000 90 1.0000
learnlayer 1.0000 1.0000 1.0000
traintol 0.0020 0.0020 0.8000 100
testtol 0.0020
maxruns 259
smoothing 0.9000 0.9000 0.9000
testruns 259
function hidden1 sigmoid 0.0000 1.0000 0.0000 1.0000
function hidden2 sigmoid 0.0000 1.0000 0.0000 1.0000
function output sigmoid 0.0000 1.0000 0.0000 1.0000
dictionary input int gen lab xray
dictionary output time
outputfile fedtst.out number none number number none 0 0 0
scale input minimum
0.000 0.000 0.000 0.000
scale input maximum
150.00 158.00 72.000 100.00
scale output minimum
69.010
scale output maximum
366.57
statistics 209790 202263 259
weigh 4 1 4 4 4 1
 1.6934 0.7606 0.3350 3.9244 -7.8650
-0.0602 -0.1542 -0.3926 -1.3950 0.5232
-7.9690 -7.9422 -7.3934 -5.2976 -7.9124
 7.9994 7.9994 7.9994 7.9994 7.9994

-7.9998 5.0866 7.9994 0.9876 -4.0502
-0.0772 -0.4270 7.9994 0.6944 -2.4110
 7.9994 7.9994 -7.9998 7.9994 7.9994
-7.9998 -7.9940 -4.9252 0.6434 6.3642

-2.9682 1.5146 0.8182 -3.3974 1.8776
```

Figure C4 Trained Brainmaker File for Predicting Mean Time in the ED($\overline{T}$) Using Individual Replications (PM 4)

```
input number 1 4
output number 1 1
hidden 7 7

filename trainfacts ef.fct
filename testfacts ef.tst
filename trainstats fef.sts
filename teststats fef.sta
learnrate  1.0000 50  1.0000 75  1.0000 90  1.0000
learnlayer  1.0000  1.0000  1.0000
traintol  0.002  0.002  0.8000 100
testtol  0.002
maxruns 5000
smoothing  0.9000  0.9000  0.9000
testruns 1

function hidden1 sigmoid  0.0000  1.0000  0.0000 1.0000
function hidden2 sigmoid  0.0000  1.0000  0.0000 1.0000
function output sigmoid  0.0000  1.0000  0.0000 1.0000
dictionary input int gen lab xray
dictionary output time
display network progress
scale input minimum
0.000 0.000 0.000 0.000
scale input maximum
150.00 158.00 72.000 100.00
scale output minimum
-32.41
scale output maximum
397.77
statistics 0 0 0
```

Figure C5 Initial Brainmaker File for Predicting Variance of Mean Time in the ED

```
weights 4 1 4 7 7 1
-1.2012  0.4802  2.3716  2.4470 -3.4860
-0.2486  0.1782  0.5914 -3.0934  0.2502
 4.4116 -5.2132 -1.1560 -0.7960  2.2680
 3.0090 -2.0234  1.7990  0.0904  2.0090
 0.1612 -1.1664  1.0076  3.3370  1.3286
-1.9856 -1.7714 -0.3244 -1.3322 -0.6422
-2.6060 -3.8554 -0.4276 -0.3262  0.9382

-0.6940  2.9596  1.1802 -2.4536  2.2350 -1.0024 -0.2620 -2.4334
-1.3670  0.1374 -0.5940  2.1702  3.5910 -3.2446 -0.1334 -2.1874
-0.3834  1.4320  0.0342  0.2250 -1.5112 -0.5366 -0.1864 -2.1500
 0.6122 -1.6502 -1.6662 -0.4304  0.3116 -2.2530  1.0256  1.1166
 1.7462  0.0726 -1.5974  4.5234 -4.0726  1.6724  1.4184 -3.0916
 1.3740 -1.8884  0.8086 -0.0316 -1.2844 -1.6716  0.6752  1.0392
 1.3886  1.6466 -2.7212 -2.7050 -0.9208 -2.2182  0.2442  1.0386

 3.6804 -3.1176 -1.0140  2.5936  3.3296  1.2604 -1.9570  2.1126
```

Figure C5 (Continued) Initial Brainmaker File for Predicting Variance of Mean Time in the ED

```
input number 1 4
output number 1 1
hidden 7 7

filename trainfacts ef.fct
filename testfacts ef.tst
filename trainstats fef.sts
filename teststats fef.sta


learnrate  1.0000 50  1.0000 75  1.0000 90  1.0000
learnlayer  1.0000  1.0000  1.0000
traintol  0.0020  0.0020  0.8000 100
testtol  0.0020
maxruns 4853
smoothing  0.9000  0.9000  0.9000
testruns 4853


function hidden1 sigmoid  0.0000  1.0000  0.0000 1.0000
function hidden2 sigmoid  0.0000  1.0000  0.0000 1.0000
function output sigmoid  0.0000  1.0000  0.0000 1.0000

dictionary input int gen lab xray

dictionary output time

outputfile feftst.out number none  number number none  0 0 0
scale input minimum
0.000 0.000 0.000 0.000
scale input maximum
150.00 158.00 72.000 100.00
scale output minimum
-32.41
scale output maximum
397.77

statistics 393093 374111 4853
```

Figure C6 Trained Brainmaker File for Predicting Variance of Mean Time in the ED

```
weights 4 1 4 7 7 1
 2.2360  5.3342 -2.8830 -6.9680 -1.8690
 1.8732  2.6390  1.9072  2.6022 -5.3666
 3.4466  7.8924  0.4372  6.9984 -2.0466
-3.4256 -0.4492 -1.3308 -4.3000  7.4470
 1.2484 -7.1686 -5.9622  1.7134  6.9882
-4.5916 -0.1308  3.7824 -0.0594 -3.5102
-0.4242 -0.7612 -1.5626  0.2506 -4.0252

 4.7486 -7.9998  5.3914  7.9762  5.9512  3.2930  7.9994 -5.2494
-7.9998  7.9994  7.9994  7.9994  7.9994 -1.9152 -7.9998  7.9994
-2.7824  1.4506  3.5470 -6.3616 -1.5336 -1.6094 -7.9998 -4.3030
-2.3386 -6.4708  1.5282 -7.8610 -1.4908  0.7952 -7.9998  3.1206
-3.9562 -0.9952  1.4812  1.9042  1.2824 -5.0970 -7.9998 -7.4362
-2.1220  5.9312  0.8676  0.0552 -1.6574 -2.9076 -7.9998 -5.9224
 1.4394 -5.6340 -5.3506 -6.3652 -7.9998  5.2662  7.9994 -4.5742

 4.4466  0.2182  7.3350  7.4608  7.9994  7.4916 -7.9998 -6.8534
```

Figure C6 (Continued) Trained Brainmaker File for Predicting Variance of Mean Time in the ED

Table C3 ANN Test Set Results for Mean Time in the ED ($\overline{T}$)

Input Parameters				Direct Simulation			ANN	
ICBWT	GCBWT	LABT	XRAYT	SIM100	Sim 1	Sim 2	PM 1	PM 4
12	12.64	5.76	8	115.3	118.72	117.84	117.4	114.8
12	12.64	5.76	92	152.7	154.04	151.76	152.6	154.6
12	12.64	66.24	8	123.8	120.20	118.31	124.5	121.6
12	12.64	66.24	92	161.8	159.06	166.63	160.3	162.9
12	145.36	5.76	8	119.6	118.18	122.34	120	118.8
12	145.36	5.76	92	157	155.83	157.39	158.3	159
12	145.36	66.24	8	128.8	133.93	138.41	128.4	124.6
12	145.36	66.24	92	169.5	166.83	169.79	165.2	166.7
138	12.64	5.76	8	119.5	121.13	124.58	119	119.9
138	12.64	5.76	92	156.5	169.53	156.79	163.6	160.6
138	12.64	66.24	8	128.2	122.43	125.99	126.7	126.1
138	12.64	66.24	92	165.7	176.64	173.37	170.5	168
138	145.36	5.76	8	124.8	126.38	128.06	122.2	122.8
138	145.36	5.76	92	164	159.44	170.53	173.2	164.5
138	145.36	66.24	8	132.8	140.13	135.47	131.4	129.9
138	145.36	66.24	92	180.6	182.43	186.43	178.2	171.1
24.75	26.07	11.88	16.5	118.8	115.49	122.28	120.8	119.9
24.75	26.07	11.88	83.5	150.4	158.70	148.85	150.6	152.1
24.75	26.07	60.12	16.5	126.2	125.36	126.55	127.5	124.9
24.75	26.07	60.12	83.5	154.9	158.22	157.56	157.2	159.1
24.75	131.93	11.88	16.5	124.9	136.26	118.45	123.4	122.4
24.75	131.93	11.88	83.5	158.3	153.60	153.14	155.2	155.8
24.75	131.93	60.12	16.5	129.6	124.64	136.11	130.9	127.7
24.75	131.93	60.12	83.5	162.6	159.19	155.57	161.3	162.4
125.25	26.07	11.88	16.5	123.3	126.16	123.67	122.5	123.3
125.25	26.07	11.88	83.5	155.9	157.85	159.36	158.3	157.1
125.25	26.07	60.12	16.5	129.9	127.92	136.58	129.6	128.9
125.25	26.07	60.12	83.5	163	156.84	153.56	164.7	163.6
125.25	131.93	11.88	16.5	127.4	129.39	132.74	125.7	125.9
125.25	131.93	11.88	83.5	162.5	157.09	156.65	165.4	160.4
125.25	131.93	60.12	16.5	136.3	131.54	137.29	133.6	132.2
125.25	131.93	60.12	83.5	170	163.01	164.19	170.8	166.6
37.5	39.5	18	25	125.5	128.98	125.14	125.1	124.3
37.5	39.5	18	75	152.2	141.98	147.15	148.7	149.6
37.5	39.5	54	25	129.6	132.68	131.72	130.8	128.6
37.5	39.5	54	75	153	150.53	149.95	154	154.9
37.5	118.5	18	25	129.3	129.39	127.38	127.5	126.5
37.5	118.5	18	75	150.6	148.51	160.40	152	152.3
37.5	118.5	54	25	134.3	132.82	128.36	133.6	130.9
37.5	118.5	54	75	159.3	166.34	151.87	157.1	157.6

Table C3(Continued) ANN Test Set Results for Mean Time in the ED ($\overline{T}$)

Input Parameters				Direct Simulation			ANN	
ICBWT	GCBWT	LABT	XRAYT	SIM100	Sim 1	Sim 2	PM 1	PM 4
112.5	39.5	18	25	129.1	128.46	131.74	126.7	127.2
112.5	39.5	18	75	150.1	150.60	155.34	153.7	153.3
112.5	39.5	54	25	132	134.01	131.71	132.8	131.9
112.5	39.5	54	75	157	151.49	148.36	158.9	158.6
112.5	118.5	18	25	130.7	132.41	136.47	129.6	129.5
112.5	118.5	18	75	155.8	165.01	153.81	158.3	156.1
112.5	118.5	54	25	136.7	135.96	135.07	135.8	134.4
112.5	118.5	54	75	161	163.55	153.65	163.2	161.1
50.25	52.93	24.12	33.5	132.2	133.54	129.80	130.4	129.5
50.25	52.93	24.12	66.5	145	149.60	148.53	146.6	146.9
50.25	52.93	47.88	33.5	136.4	128.95	139.64	134.4	132.8
50.25	52.93	47.88	66.5	151.9	145.93	157.41	150.4	150.6
50.25	105.07	24.12	33.5	135.2	128.61	136.85	132.3	131.2
50.25	105.07	24.12	66.5	148.2	139.05	137.91	148.8	148.8
50.25	105.07	47.88	33.5	136.5	131.65	147.71	136.3	134.4
50.25	105.07	47.88	66.5	154	147.45	157.15	152.5	152.5
99.75	52.93	24.12	33.5	134.8	140.00	135.41	131.9	131.8
99.75	52.93	24.12	66.5	148.2	145.18	146.61	149.4	149.6
99.75	52.93	47.88	33.5	135.8	134.08	142.91	135.9	135.2
99.75	52.93	47.88	66.5	154.5	150.92	157.50	153.2	153.2
99.75	105.07	24.12	33.5	135.2	147.06	141.10	133.9	133.4
99.75	105.07	24.12	66.5	152	148.09	146.73	152.1	151.3
99.75	105.07	47.88	33.5	140.3	136.64	150.72	138	136.9
99.75	105.07	47.88	66.5	153.1	151.78	162.78	155.7	154.9
63	66.36	30.24	42	140.2	135.60	139.67	136.4	135.6
63	66.36	30.24	58	148.1	151.29	159.34	144.4	144.3
63	66.36	41.76	42	139.5	141.03	142.72	138.3	137.3
63	66.36	41.76	58	146.2	148.93	145.67	146.4	146.1
63	91.64	30.24	42	140.4	132.58	142.12	137.3	136.5
63	91.64	30.24	58	145.1	137.93	147.58	145.5	145.2
63	91.64	41.76	42	139.4	142.40	135.70	139.2	138.1
63	91.64	41.76	58	147.1	152.47	142.56	147.4	146.9
87	66.36	30.24	42	138.7	137.70	138.53	137.2	136.8
87	66.36	30.24	58	146.4	155.15	145.32	145.6	145.6
87	66.36	41.76	42	141.8	148.54	140.33	139.2	138.4
87	66.36	41.76	58	149.4	148.85	144.07	147.6	147.3
87	91.64	30.24	42	136.6	148.30	130.09	138.2	137.6
87	91.64	30.24	58	144.8	148.13	146.34	146.8	146.4
87	91.64	41.76	42	140	142.01	143.44	140.2	139.5
87	91.64	41.76	58	151.8	148.60	146.93	148.7	148.3

Table C4 ANN Test Set Results for Variance of Mean Time in ED ($Var(\overline{T})$)

Input Parameters				Direct Simulation			ANN
ICBWT	GCBWT	LABT	XRAYT	SIM100	Sim 1	Sim 2	
12	12.64	5.76	8	10.16	11.11	11.68	15.62
12	12.64	5.76	92	35.47	104.48	26.42	27.80
12	12.64	66.24	8	16.15	18.97	5.54	13.52
12	12.64	66.24	92	72.86	59.98	54.75	14.68
12	145.36	5.76	8	11.84	5.21	5.77	11.63
12	145.36	5.76	92	27.28	9.64	38.79	24.65
12	145.36	66.24	8	17.62	19.21	29.97	13.10
12	145.36	66.24	92	57.32	52.97	55.70	58.79
138	12.64	5.76	8	12.26	9.22	27.05	14.15
138	12.64	5.76	92	24.44	85.62	25.04	35.79
138	12.64	66.24	8	11.73	16.51	11.11	22.03
138	12.64	66.24	92	44.4	114.29	25.55	55.21
138	145.36	5.76	8	12.47	37.84	17.26	11.63
138	145.36	5.76	92	46.29	32.32	74.07	48.18
138	145.36	66.24	8	13.73	20.42	11.41	28.33
138	145.36	66.24	92	97.96	77.32	133.74	193.00
24.75	26.07	11.88	16.5	11.63	4.35	7.31	20.03
24.75	26.07	11.88	83.5	27.8	40.83	25.76	27.70
24.75	26.07	60.12	16.5	13.73	7.65	8.50	16.15
24.75	26.07	60.12	83.5	25.49	13.59	27.88	16.67
24.75	131.93	11.88	16.5	16.46	17.21	6.56	11.94
24.75	131.93	11.88	83.5	57.11	11.82	30.98	24.02
24.75	131.93	60.12	16.5	15.83	9.93	24.52	14.89
24.75	131.93	60.12	83.5	55.84	4.26	26.52	68.03
125.25	26.07	11.88	16.5	17.62	30.32	9.33	16.67
125.25	26.07	11.88	83.5	39.04	61.49	23.61	27.17
125.25	26.07	60.12	16.5	12.15	3.94	17.01	22.55
125.25	26.07	60.12	83.5	40.93	56.25	9.12	37.89
125.25	131.93	11.88	16.5	13.42	15.72	34.68	11.63
125.25	131.93	11.88	83.5	29.8	11.18	25.05	37.99
125.25	131.93	60.12	16.5	18.25	24.50	11.10	25.60
125.25	131.93	60.12	83.5	45.97	29.13	86.56	16.99
37.5	39.5	18	25	17.41	17.10	7.01	23.92
37.5	39.5	18	75	28.33	7.24	29.70	27.28
37.5	39.5	54	25	17.93	10.17	9.66	19.61
37.5	39.5	54	75	38.31	14.35	39.81	19.61
37.5	118.5	18	25	17.72	8.94	19.44	12.78
37.5	118.5	18	75	32.21	19.86	38.38	23.50
37.5	118.5	54	25	20.14	8.00	6.54	17.30
37.5	118.5	54	75	34.74	43.39	39.53	52.38

Table C4(Continued) ANN Test Set Results for Variance of Mean Time in ED ($Var(\overline{T})$)

Input Parameters				Direct Simulation			ANN
ICBWT	GCBWT	LABT	XRAYT	SIM100	Sim 1	Sim 2	
112.5	39.5	18	25	18.04	18.28	8.55	19.40
112.5	39.5	18	75	29.9	13.13	24.25	25.18
112.5	39.5	54	25	14.78	13.81	12.96	22.76
112.5	39.5	54	75	33.89	12.64	10.80	28.64
112.5	118.5	18	25	18.88	10.23	27.18	11.94
112.5	118.5	18	75	61.73	103.70	26.81	29.38
112.5	118.5	54	25	26.86	15.95	13.04	23.60
112.5	118.5	54	75	44.71	43.59	17.59	46.60
50.25	52.93	24.12	33.5	11.94	12.14	13.84	24.86
50.25	52.93	24.12	66.5	19.93	21.64	20.90	26.54
50.25	52.93	47.88	33.5	24.65	13.23	12.51	21.92
50.25	52.93	47.88	66.5	25.91	12.92	100.66	22.13
50.25	105.07	24.12	33.5	21.5	9.50	20.79	15.73
50.25	105.07	24.12	66.5	17.72	9.68	20.77	23.29
50.25	105.07	47.88	33.5	19.51	10.31	39.66	18.77
50.25	105.07	47.88	66.5	34.31	11.60	19.78	31.37
99.75	52.93	24.12	33.5	22.13	9.19	12.47	21.71
99.75	52.93	24.12	66.5	42.3	31.18	17.73	24.97
99.75	52.93	47.88	33.5	15.52	7.75	65.31	22.66
99.75	52.93	47.88	66.5	34.84	39.34	54.84	25.60
99.75	105.07	24.12	33.5	15.94	21.31	17.10	13.84
99.75	105.07	24.12	66.5	39.15	12.71	14.17	24.86
99.75	105.07	47.88	33.5	25.18	12.47	39.05	21.29
99.75	105.07	47.88	66.5	20.98	20.04	53.79	53.95
63	66.36	30.24	42	22.24	25.02	18.76	23.92
63	66.36	30.24	58	39.15	38.49	86.18	24.97
63	66.36	41.76	42	25.6	19.53	19.75	22.66
63	66.36	41.76	58	22.55	14.63	11.69	23.50
63	91.64	30.24	42	24.23	4.99	19.72	19.93
63	91.64	30.24	58	23.18	16.22	21.60	22.97
63	91.64	41.76	42	14.68	11.22	14.48	20.45
63	91.64	41.76	58	20.87	9.09	13.55	23.71
87	66.36	30.24	42	23.39	15.04	12.92	22.87
87	66.36	30.24	58	26.86	84.82	17.91	24.44
87	66.36	41.76	42	29.8	43.30	26.79	22.87
87	66.36	41.76	58	27.7	20.80	24.97	24.34
87	91.64	30.24	42	22.24	18.80	9.53	18.98
87	91.64	30.24	58	32.32	76.16	21.29	23.18
87	91.64	41.76	42	20.87	23.87	30.68	20.77
87	91.64	41.76	58	30.22	16.28	12.78	26.23

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